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***PT* symmetry of the non-Hermitian XX spin-chain: non-local bulk interaction from complex boundary fields**

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Abstract

The XX spin-chain with non-Hermitian diagonal boundary conditions is shown to be quasi-Hermitian for special values of the boundary parameters. This is proved by an explicit construction of a new inner product employing a ‘quasi-fermion’ algebra in momentum space, where creation and annihilation operators are not related via Hermitian conjugation. For a special example, when the boundary fields lie on the imaginary axis, we show the spectral equivalence of the quasi-Hermitian XX spin-chain with a non-local fermion model, where long-range hopping of the particles occurs as the non-Hermitian boundary fields increase in strength. The corresponding Hamiltonian interpolates between the open XX and the quantum group invariant XXZ model at the free fermion point. For an even number of sites the former is known to be related to a CFT with central charge $c = 1$, while the latter has been connected to a logarithmic CFT with central charge $c = -2$. We discuss the underlying algebraic structures and show that for an odd number of sites the superalgebra symmetry $U(\mathfrak{gl}(1|1))$ can be extended from the unit circle along the imaginary axis. We relate the vanishing of one of its central elements to the appearance of Jordan blocks in the Hamiltonian.

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1. Introduction

Recent years have seen increasing interest in non-Hermitian quantum Hamiltonians H and how to give them a physical sound interpretation. In this paper we revisit an exactly-solvable, one-

dimensional, discrete system, the XX-Hamiltonian with non-Hermitian diagonal boundary conditions, i.e.

$$H = \frac{1}{2} \sum_{m=1}^{M-1} [\sigma_m^x \sigma_{m+1}^x + \sigma_m^y \sigma_{m+1}^y] + \frac{\alpha \sigma_1^z + \beta \sigma_M^z}{2}, \quad \alpha, \beta \in \mathbb{C}. \quad (1)$$

Here, $\sigma_m^{x,y,z}$ denote the Pauli matrices acting in the m th copy of an M -fold tensor product $V^{\otimes M}$ of a two-dimensional complex vector space $V = \mathbb{C}v_+ \oplus \mathbb{C}v_-$. For real values the parameters $\alpha, \beta \in \mathbb{R}$ have the physical interpretation of external magnetic fields located at the boundary. Here we are interested in investigating the case of *complex* fields, $\alpha, \beta \in \mathbb{C}$. Another variant of the XX-Hamiltonian we shall consider is

$$H' = \frac{1}{2} \sum_{m=1}^{M-1} [\sigma_m^x \sigma_{m+1}^x + \sigma_m^y \sigma_{m+1}^y - \beta \sigma_m^z - \alpha \sigma_{m+1}^z] = H - \frac{\alpha + \beta}{2} \sum_{m=1}^M \sigma_m^z \quad (2)$$

which up to boundary terms coincides with the closed or periodic XX spin-chain Hamiltonian in an external magnetic field. Both Hamiltonians can be diagonalized via a Jordan–Wigner transformation for arbitrary complex values of the boundary parameters α, β . However, the Hamiltonians H, H' with $\alpha, \beta \in \mathbb{C}$ are in general non-Hermitian,

$$H \neq H^* = H(\bar{\alpha}, \bar{\beta}), \quad (3)$$

and one needs to explain how a meaningful quantum-mechanical system in terms of H, H' can be defined. On physical grounds the time evolution operator $U(t) = \exp(itH), t > 0$, ought to be unitary and, hence, H needs to be Hermitian. Thus, a non-Hermitian Hamiltonian, $H \neq H^*$, appears at first sight to be in contradiction with conventional quantum mechanics. However, under certain assumptions, the Hamiltonian might turn out to be quasi-Hermitian [1, 2]. That is, there exists a *positive, Hermitian and invertible* operator η satisfying

$$\eta H = H^* \eta. \quad (4)$$

This allows one to either introduce a new inner product,

$$\langle v, w \rangle_\eta := \langle v, \eta w \rangle, \quad v, w \in \mathfrak{H} \quad (5)$$

on the state space \mathfrak{H} with respect to which H becomes Hermitian or perform a similarity transformation to a new, Hermitian Hamiltonian with respect to the original inner product,

$$h = \eta^{1/2} H \eta^{-1/2}. \quad (6)$$

Given a non-Hermitian Hamiltonian, it is in general rather difficult to determine whether it is quasi-Hermitian. A special subclass of quasi-Hermitian systems where this turns out to be easier is that distinguished by PT symmetry, i.e. Hamiltonian systems where the eigenvectors can be chosen such that they are eigenvectors under a joint parity and time-reversal transformation; see, e.g. [3] and references therein. In this case, the quasi-Hermiticity operator η enjoys further constraints which we will discuss in the text below. Employing the exact solvability of the non-Hermitian XX spin-chain, we will establish for which values of the boundary parameters it is quasi-Hermitian and show its PT symmetry.

1.1. Long-range bulk interaction from non-Hermitian boundary fields

The above non-Hermitian Hamiltonians are of special interest because of their underlying algebraic structure and we will show that it plays an important role in the interpretation of the new inner product. Setting $\alpha = -\beta = \sqrt{-1}$, the Hamilton (1) is the $U_q(sl_2)$ -invariant XXZ spin-chain evaluated at the free fermion point $q = \sqrt{-1}$ [4, 5]. In the thermodynamic limit

it has been suggested [6–8] that this discrete system is closely connected with critical dense polymers effectively described by a logarithmic conformal field theory with central charge $c = -2$ (see, e.g. [9, 10] for reviews). Moreover, it has been stressed that the corresponding lattice models should be described in terms of non-local statistical degrees of freedom, such as ‘connectivities’; see, e.g. [7].

On the other hand, setting $\alpha = \beta = 0$, chain (1) becomes Hermitian and is related to the Ashkin–Teller model, see [4]. In the thermodynamic limit the system is now described by an ordinary conformal field theory with central charge $c = 1$.

Thus, the non-Hermitian Hamiltonian,

$$H_g = \frac{1}{2} \sum_{m=1}^{M-1} [\sigma_m^x \sigma_{m+1}^x + \sigma_m^y \sigma_{m+1}^y + ig(\sigma_m^z - \sigma_{m+1}^z)] = H_{-g}^*, \quad 0 < g < 1, \quad (7)$$

interpolates between these two special cases. We will show for small values of the coupling constant g its spectral equivalence with the Hermitian Hamiltonian

$$h_{g^2} = - \sum_{n>0} \sum_{x=1}^{M-n} p_x^{(n)}(g^2) [c_x^* c_{x+n} - c_x c_{x+n}^*], \quad (8)$$

where c_x^* and c_x are fermionic creation and annihilation operators at lattice site x . The hopping probability between a site x and its n th neighbour is encoded in the real coefficients $p_x^{(n)}$ which only depend on g^2 and vanish for n even, $p_x^{(2n)} = 0$. At $g = 0$ we only have nearest-neighbour hopping,

$$h_0 = - \sum_{x=1}^{M-1} (c_x^* c_{x+1} - c_x c_{x+1}^*). \quad (9)$$

Our perturbative calculation will show that as g increases the bulk interaction becomes more and more long-range by successively ‘switching on’ the various coefficients $p_x^{(2n+1)}$ starting from the boundary sites $x = 1, M$. More precisely, we find up to order g^8 that the non-vanishing contributions are

$$\begin{aligned} p_x^{(1)} &= 1 - \frac{128g^2 + 8g^4 + g^6}{512} (\delta_{x,1} + \delta_{x,M-1}) \\ &\quad - \frac{8g^4 + 3g^6}{512} (\delta_{x,2} + \delta_{x,M-2}) + \frac{g^6}{256} (\delta_{x,3} + \delta_{x,M-3}) + O(g^8), \\ p_x^{(3)} &= \frac{20g^4 + 3g^6}{256} (\delta_{x,1} + \delta_{x,M-3}) + \frac{5g^6}{512} (\delta_{x,2} + \delta_{x,M-4}) + O(g^8), \\ p_x^{(5)} &= -\frac{23g^6}{512} (\delta_{x,1} + \delta_{x,M-5}) + O(g^8). \end{aligned} \quad (10)$$

Figure 1 indicates which hopping amplitudes, i.e. the probabilities for a fermion to jump between two lattice sites, are modified up to order g^8 . We have only depicted the additional contributions for $g > 0$: whenever an arc connects two lattice sites x and $x + n$ then there is a non-vanishing coefficient $p_x^{(n)}$.

Both variants (7) and (8) of the Hamiltonian have their advantages:

- The Hermitian Hamiltonian h serves physical intuition. It can be directly interpreted and clearly shows the long-range nature of the interaction which is not apparent in (7). It suggests that the long-range nature of the interaction with increasing g is behind the singular change from an ‘ordinary’ conformal field theory with $c = 1$ for $0 \leq g < 1$ to a logarithmic one with $c = -2$ at $g = 1$.

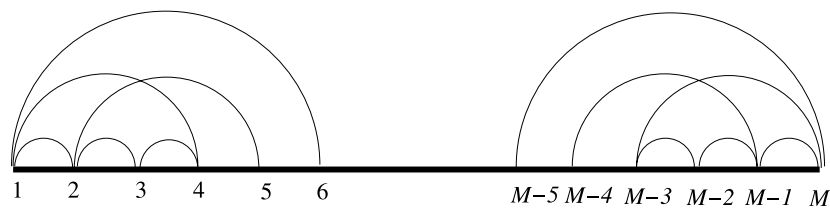


Figure 1. Graphical depiction of the long-range hopping.

- In contrast, variant (7) highlights the algebraic properties, such as integrability and quantum group invariance. The PT symmetry and quasi-Hermiticity of the quantum group invariant XXZ spin-chain for higher roots of unity $q = \exp(i\pi/r)$, $r > 2$, have been discussed in another paper [11].

Note that the appearance of a long-range bulk interaction does not contradict physical intuition. Naively one would argue that boundary terms will become unimportant in the thermodynamic limit when the number of sites tends to infinity. However, the applicability of this statement crucially depends on the nature of the boundary conditions, see for instance [12]. In this paper we consider a different, novel example of this phenomenon. The complex boundary terms render the Hamiltonian non-Hermitian, hence they imply a drastic non-local change in the mathematical structure of the state space: the introduction of a new inner product. We will see that this is the case by observing that the similarity transformation which maps H_g into h_{g^2} is highly non-local.

1.2. Outline of the paper and summary of results

The purpose of this paper is to relate the notions of PT symmetry and quasi-Hermiticity to another simple but non-trivial model. While the XX spin-chain with non-Hermitian boundary terms has been discussed previously in the literature (see, e.g. [13–17]), it has not been investigated for which parameter values α, β the Hamiltonian is quasi-Hermitian and what the corresponding Hermitian systems are. We will show that for $\alpha = \bar{\beta}$ inside the unit disc the Hamiltonians (1) and (2) are quasi-Hermitian, this condition on α, β ensures also PT symmetry. We will then discuss for which values the mentioned Hamiltonians cease to be quasi-Hermitian and when their spectrum contains complex eigenvalues. The special case $\alpha = \bar{\beta}$ of the non-Hermitian XX spin-chain, which includes (7), has not been discussed in detail previously.

For the benefit of the reader, we summarize the new results contained in this paper.

- After a brief review of the notions of quasi-Hermiticity and PT symmetry on the lattice in section 2, we establish in section 3 that the spectra of the Hamiltonians (1) and (2) are real for boundary parameters within the unit disc, $\alpha = \bar{\beta} \in \mathbb{C}$ and $|\alpha| < 1$. Performing a Jordan–Wigner transformation the XX spin-chain can be reformulated as a non-trivial fermion model and its spectrum can be described in terms of quasi-particle excitations in momentum space. We will give an elementary proof that all quasi-momenta (Bethe roots) lie on the unit circle and state for $\alpha = -\beta = ig$, $0 < g < 1$ a set of palindromic polynomials whose roots give the quasi-momenta k and the associated energies $2 \cos k$.
- In section 4 we highlight that unlike in the case of real boundary fields $\alpha, \beta \in \mathbb{R}$, the Jordan–Wigner transformation does *not* lead to a well-defined fermion algebra in

momentum space, but instead one has two sets $\{\hat{c}_k^*, \hat{c}_k\}$ and $\{\hat{d}_k^*, \hat{d}_k\}$ of creation and annihilation operators which satisfy the relations

$$[\hat{c}_k^*, \hat{d}_{k'}]_+ = \delta_{k,k'}, \quad [\hat{c}_k, \hat{d}_{k'}]_+ = [\hat{c}_k^*, \hat{d}_{k'}^*]_+ = 0, \quad \hat{c}_k^* \neq \hat{d}_k. \quad (11)$$

Here, $k = -i \ln z \in \mathbb{R}$ is a quasi-momentum, $[A, B]_+ = AB + BA$ is the anti-commutator and $*$ denotes the Hermitian adjoint with respect to the original inner product, where the Hamiltonian is non-Hermitian. Employing the above operators we explicitly construct an η which not only renders the Hamiltonian Hermitian but obeys the more restrictive condition

$$\eta \hat{c}_k^* = \hat{d}_k^* \eta \quad \text{and} \quad \eta \hat{d}_k = \hat{c}_k \eta. \quad (12)$$

That is, with respect to the new inner product (5) $\{\hat{c}_k^*, \hat{d}_k\}$ satisfy the canonical anti-commutation relations *and* are the Hermitian adjoint of each other.

- Also in section 4 we extend for $\alpha = -\beta = ig, 0 \leq g \leq 1$, the well-known $U_{q=i}(sl_2)$ symmetry of (7) from the unit circle, $g = 1$, into the unit disc, $0 \leq g < 1$ and discuss the invariance of the Hamiltonian for odd and even number of sites. Both cases show remarkable differences. The quantum group symmetry is closely connected with so-called fermionic zero modes and we show that at the coupling values g where the anticommutator of the associated fermionic creation and annihilation operators vanishes the Hamiltonian possesses non-trivial Jordan blocks. Thus, the Hamiltonian ceases to be quasi-Hermitian. For even numbers of sites this happens at $g = 1$, i.e. on the unit circle, as was observed previously [7]. Here we show that it also happens for odd numbers of sites albeit at the value $g_{\max} = \sqrt{(M+1)/(M-1)}$ which approaches the value 1 in the limit $M \rightarrow \infty$. It also signals the onset of complex eigenvalues for values of $g > g_{\max}$, i.e. outside the unit disc.
- In section 5 we present a perturbative calculation of η in terms of the coupling parameter $0 < g \ll 1$ in (7). While we follow closely the steps previously put forward in the literature [18, 19], we give a novel derivation of the coefficients in the perturbation series expansion. Using these results we obtain expression (7). We will also derive some closed expressions for a small number of sites $M = 3, 4$ and 5 in section 6. For $g = 1$ and odd lattice sites we formulate a conjecture on an alternative way of computing the new inner product using the Temperley–Lieb algebra.
- In section 7 we will investigate briefly the case of general complex boundary fields inside the unit disc, i.e. when $\alpha = \bar{\beta} = g e^{i\theta}$ with $\theta \neq \pi/2$ and real in order to make contact with the discussion in [13].
- Section 8 contains the conclusions.

2. Quasi-Hermiticity and PT invariance

The state space of the non-Hermitian systems (1) and (2) is a spin-chain of M sites represented in terms of the tensor product $V^{\otimes M}$ of the two-dimensional complex vector space V with orthonormal basis $\{v_{\pm}\}$ such that $\sigma^z v_{\pm} = \pm v_{\pm}$. The tensor product is then spanned by the vectors

$$\{|\varepsilon_1, \dots, \varepsilon_M\rangle \equiv v_{\varepsilon_1} \otimes \dots \otimes v_{\varepsilon_M} : \varepsilon_m = \pm 1\}. \quad (13)$$

This particular choice of basis vectors is motivated by the axial symmetry of the Hamiltonians H, H' which commute with the total spin operator,

$$S^z = \frac{1}{2} \sum_{m=1}^M \sigma_m^z, \quad [H, S^z] = [H', S^z] = 0. \quad (14)$$

The matrices (1) and (2) are defined with respect to the inner product

$$\langle \varepsilon_1, \dots, \varepsilon_M | \varepsilon'_1, \dots, \varepsilon'_M \rangle = \prod_{i=1}^M \langle v_{\varepsilon_i}, v_{\varepsilon'_i} \rangle, \quad \langle v_{\varepsilon}, v_{\varepsilon'} \rangle = \delta_{\varepsilon\varepsilon'}. \quad (15)$$

As already pointed out in the introduction both Hamiltonians, H and H' , are in general non-Hermitian for arbitrary complex boundary parameters α, β . However, in the above basis (13) both of them are symmetric,

$$H = H^t \quad \text{and} \quad H' = H'^t.$$

We now wish to determine for which values there exists a map $\eta : V^{\otimes M} \rightarrow V^{\otimes M}$ possessing the following properties:

- (1) η is Hermitian, $\eta = \eta^*$, invertible, $\det \eta > 0$, and positive definite, $\eta > 0$;
- (2) η intertwines the Hamiltonian H (respectively H') with its Hermitian adjoint,

$$\eta H = H^* \eta. \quad (16)$$

Because of the axial symmetry present in H and H' we add the following requirement which implies that η intertwines H and H' at the same time,

$$[\eta, S^z] = 0. \quad (17)$$

Provided that such a map η exists we define a new inner product and with it a new Hilbert space structure via

$$\langle v, w \rangle_{\eta} := \langle v, \eta w \rangle, \quad v, w \in V^{\otimes M}. \quad (18)$$

Using the intertwining property (2) it is obvious that the Hamiltonian is Hermitian with respect to the new inner product. The properties listed under (1) ensure that the new inner product is well defined.

There is an alternative to introducing a new Hilbert space structure. Since $\eta > 0$ it follows that there exists a unique positive definite square root $\eta^{\frac{1}{2}} > 0$ which allows one to define the Hermitian Hamiltonian

$$h = \eta^{\frac{1}{2}} H \eta^{-\frac{1}{2}} \quad (19)$$

with respect to the original inner product.

Both approaches have their advantages and disadvantages. At first glance one might prefer to work in the original Hilbert space with the ‘gauge-transformed’ Hamiltonian h , as this allows for a direct physical interpretation without having to insert another operator when taking scalar products. However, for practical purposes it is often more feasible to work with H and η . Even if it is possible to construct η explicitly, the computation of its square root and, thus, the calculation of h is another technically complicated step. We will perform this computation for (7) to low orders in g employing perturbation theory in section 5. In contrast, the original Hamiltonian H has usually a simpler form which allows one to read off certain symmetries. The XX-chain with imaginary boundary fields is a concrete example.

2.1. Parity, time and spin reversal on the lattice

On the set of basis vectors (13) we define the parity-reversal operator P by

$$P|\varepsilon_1, \dots, \varepsilon_M\rangle = |\varepsilon_M, \varepsilon_{M-1}, \dots, \varepsilon_1\rangle \quad (20)$$

and extend its action to the whole space by linearity. From this definition, it is immediate to see that

$$PHP = H(\beta, \alpha). \quad (21)$$

The time-reversal operator T acts on the basis vectors as identity,

$$T|\varepsilon_1, \dots, \varepsilon_M\rangle = |\varepsilon_1, \dots, \varepsilon_M\rangle, \quad (22)$$

but is defined to be *antilinear*, whence any matrix (such as the Hamiltonian) is transformed into its complex conjugate under the adjoint action of T ,

$$THT = \bar{H} = H(\bar{\alpha}, \bar{\beta}) = H^*. \quad (23)$$

Below we will define discrete wavefunctions which will be transformed into their complex conjugates under the operator T . This justifies the identification of T with time reversal.

Upon imposing the constraint

$$\alpha = \bar{\beta} \quad (24)$$

the Hamiltonian turns out to be PT -invariant,

$$\alpha = \bar{\beta} : \quad [PT, H] = 0. \quad (25)$$

Note, however, that PT invariance of the Hamiltonian is not a sufficient criterion to ensure real eigenvalues, this only follows once it is established that the eigenvectors of the Hamiltonian can be chosen to be simultaneously eigenvectors of the PT operator. This is not automatically implied by PT invariance of the Hamiltonian as the time-reversal T is an antilinear operator; see, e.g. [20].

For later purposes we also discuss the behaviour under the spin-reversal operator,

$$RH(\alpha, \beta)R = H(-\alpha, -\beta), \quad R = \prod_{m=1}^M \sigma_m^x. \quad (26)$$

Thus, in general spin-reversal symmetry is broken in the presence of boundary fields.

Provided that the Hamiltonian is not only PT -invariant but satisfies the slightly more restrictive constraint

$$PHP = THT = H^*, \quad (27)$$

as it is the case here for $\alpha = \bar{\beta}$, it is natural to impose further constraints on η . Namely, we wish to have

$$P\eta P = T\eta T = \eta^{-1}. \quad (28)$$

These conditions are compatible with the intertwining property, e.g.

$$P\eta HP = P\eta PH^* = HP\eta P = PH^*\eta P.$$

In essence we are demanding that parity reversal gives the same η up to inversion. The same applies for time reversal.

Often it is beneficial to define an additional operator C introduced by Bender and collaborators (for references see [3]) by setting

$$C := P\eta. \quad (29)$$

This operator might turn out to have a simpler expression than η itself. The aforementioned properties of η imply the identities

$$C^2 = 1, \quad [PT, C] = 0, \quad [H, C] = 0. \quad (30)$$

The C -operator turned out to have an elegant algebraic expression for the quantum group invariant XXZ spin-chain; see [11].

3. Spectrum and eigenvectors of the Hamiltonian

As mentioned in the introduction the Hamiltonians H, H' can be diagonalized in terms of free fermions. Using the well-known Jordan–Wigner identities

$$c_x = \left(\prod_{y < x} \sigma_y^z \right) \sigma_x^-, \quad c_x^* = \left(\prod_{y < x} \sigma_y^z \right) \sigma_x^+ \quad \text{and} \quad n_x = c_x^\dagger c_x = \frac{1 + \sigma_x^z}{2}, \quad (31)$$

we introduce fermion creation and annihilation operators in ‘position space’ satisfying the canonical anti-commutation relations (CAR),

$$[c_x, c_y]_+ = [c_x^*, c_y^*]_+ = 0 \quad \text{and} \quad [c_x^*, c_y]_+ = \delta_{x,y}, \quad x, y = 1, 2, \dots, M. \quad (32)$$

For later purposes we also state the transformation properties under parity, time and spin reversal,

$$P c_x = c_{M+1-x} P, \quad T c_x = c_x T, \quad R c_x = (-1)^{x+1} c_x^* R. \quad (33)$$

In terms of the fermion algebra the Hamiltonians can be rewritten as

$$H = - \sum_{x=1}^{M-1} [c_x^* c_{x+1} - c_x c_{x+1}^*] + \alpha n_1 + \beta n_M - \frac{\alpha + \beta}{2} \quad (34)$$

and

$$H' = - \sum_{x=1}^{M-1} \left[c_x^* c_{x+1} - c_x c_{x+1}^* + \beta n_x + \alpha n_{x+1} - \frac{\alpha + \beta}{2} \right]. \quad (35)$$

Below we shall constrain the boundary parameters α, β . For the moment we leave them arbitrary. We now introduce a ‘discrete wavefunction’ ψ_z depending on a complex parameter $z \in \mathbb{C}$ by defining

$$\hat{c}_z^* = \sum_{x=1}^M \psi_z(x; \alpha, \beta) c_x^*, \quad (36)$$

with

$$\psi_z(x; \alpha, \beta) = z^x - A(z; \alpha, \beta) z^{-x}. \quad (37)$$

This ansatz is physically motivated: it is a superposition of two (discrete) plane waves, one incoming and one reflected. Here, $z = \exp(ik)$ with k being the quasi-momentum and A is the reflection coefficient. Note that we allow here for complex momenta k .

Employing the canonical anticommutation relations one easily finds that

$$\begin{aligned} c_x^* H &= H c_x^* + c_{x-1}^* + c_{x+1}^*, & 1 < x < M, \\ c_1^* H &= H c_1^* - \alpha c_1^* + c_2^*, \\ c_M^* H &= H c_M^* + c_{M-1}^* - \beta c_M^*. \end{aligned}$$

Therefore, one has

$$[H, \hat{c}_z^*] = -(z + z^{-1}) \hat{c}_z^* \quad (38)$$

provided the coefficient A in wavefunction (37) obeys the identities [4]

$$A = \frac{1 + \alpha z}{1 + \alpha/z} = z^{2M} \frac{\beta + z}{\beta + z^{-1}}. \quad (39)$$

As both equations have to hold simultaneously this imposes a constraint on the allowed values for the parameter z which are specified as the roots of a polynomial equation of order

$2M+2$. From (38) we infer that the spectrum of the Hamiltonian is composed of quasi-particle excitations with energy $\varepsilon = z + z^{-1}$ by successively acting with (36) on the pseudo-vacuum vector $|0\rangle = v_{-1} \otimes \dots \otimes v_{-1}$,

$$H|z_1, \dots, z_l\rangle = \left(-\frac{\alpha + \beta}{2} - \sum_{i=1}^l (z_i + z_i^{-1}) \right) |z_1, \dots, z_l\rangle, \quad (40)$$

where

$$|z_1, \dots, z_l\rangle = \hat{c}_{z_1}^* \dots \hat{c}_{z_l}^* |0\rangle. \quad (41)$$

Thus, it depends on the nature of the solutions z of equation (39) whether the spectrum of the Hamiltonian is real.

Proposition 1. *Let $\alpha = \bar{\beta}$ in (1) and assume that α is inside the closed unit disc, i.e. $|\alpha| \leq 1$. Then the solutions of (39) all lie on the unit circle, hence the quasi-momenta $k_j = -i \ln z_j$ are real.*

Proof. Let us rewrite the Bethe ansatz equations (39) as

$$z^M \frac{z + \alpha}{z\bar{\alpha} + 1} = z^{-M} \frac{z^{-1} + \alpha}{z^{-1}\bar{\alpha} + 1}, \quad (42)$$

and define the maps $f(z) = z^M(z + \alpha)/(z\bar{\alpha} + 1)$ and $g(z) = f(z^{-1})$. Note that the above Bethe ansatz equations are invariant under complex conjugation and $z \rightarrow z^{-1}$, which reflects the PT invariance of the Hamiltonian. Thus, we can assume without loss of generality that there exists a solution z_0 with $|z_0| \leq 1$. For $|\alpha| \leq 1$ the image of the closed unit disc under the map f lies again in the closed unit disc. In contrast, the image of the closed unit disc under the map g lies outside of the open disc. Hence, any solution to (42) with $|\alpha| \leq 1$ must lie on the boundary of these two image regions, i.e. the unit circle. \square

Remark. Motivated by the previous proposition we shall henceforth use the parametrization

$$\alpha = \bar{\beta} = g e^{i\theta}, \quad g \geq 0 \quad (43)$$

for the boundary parameters. The Hamiltonian therefore now depends only on two real parameters, $g \geq 0$ and $0 \leq \theta < 2\pi$.

Note that there are only M relevant solutions to the Bethe ansatz equations. The trivial roots $z = \pm 1$ do not occur in the spectrum of the Hamiltonian which allows one to reduce the problem of solving (39) to finding the roots of the following palindromic or self-reciprocal polynomial

$$f(z) = z^{2M} f(z^{-1}) = z^{2M} + 1 + (1 + g^2) \sum_{m=1}^{M-1} z^{2m} + 2g \cos \theta \sum_{m=0}^{M-1} z^{2m+1}. \quad (44)$$

Thus, all roots z_i occur in reciprocal pairs and there exists a unique polynomial

$$F(\varepsilon) = \prod_{i=1}^M (\varepsilon - \varepsilon_i) \quad (45)$$

of order M whose roots are given by the single-particle energies (compare with (40))

$$\varepsilon_i = z_i + z_i^{-1}. \quad (46)$$

Note that the ambiguity in the definition of the Bethe root z_i does not matter, as wavefunction (37) is simply rescaled by changing $z_i \rightarrow z_i^{-1}$. Thus, the problem of computing the

eigenvectors and spectrum of the Hamiltonian is reduced to finding the roots ε_i of a polynomial F of degree M . For example, setting $M = 8$ and $\rho = \alpha + \beta$, $\sigma = 1 + \alpha\beta$, we obtain

$$F(\varepsilon) = \varepsilon^8 - \varepsilon^6(8 - \sigma) + 5\varepsilon^4(4 - \sigma) - 2\varepsilon^2(8 - 3\sigma) + 2 - \sigma - 4\rho\varepsilon + 10\rho\varepsilon^3 - 6\rho\varepsilon^5 + \rho\varepsilon^7. \tag{47}$$

We now specialize to the case of particular interest, $\alpha = -\beta = ig$, $g \in \mathbb{R}$, and present general expressions for the reduced polynomial F for all M .

3.1. Palindromic polynomials for purely imaginary boundary fields

For the special choice $\theta = \pm\pi/2$ the palindromic polynomial (44) simplifies since all terms involving odd powers disappear. One easily convinces oneself that this leads to the further simplification that all roots occur in pairs $\pm\varepsilon_i$. Furthermore, if the number of sites M is odd one easily verifies that one has the roots $z_i = \pm\sqrt{-1}$. The latter give rise to a ‘zero mode’, $\varepsilon_i = 0$, of the Hamiltonian

$$[H, \hat{c}_{z=i}^*] = 0,$$

where the corresponding wavefunction is given by

$$\psi_{z=i}(x) = \frac{\sin \frac{\pi x}{2} - ig \cos \frac{\pi x}{2}}{\sqrt{\frac{M+1}{2} - \frac{M-1}{2}g^2}}.$$

A similar expression holds for $z = -i$. As we will see below, this solution for the discrete wavefunction is connected with a $U(\mathfrak{gl}(1|1))$ symmetry of the Hamiltonian. Dividing out the zero mode, we end up with a palindromic polynomial of degree $2(M - 1)$,

$$f(z) = \sum_{k=0}^m z^{4k} + g^2 \sum_{k=0}^{m-1} z^{4k+2}, \quad m = \frac{M-1}{2}.$$

Setting therefore

$$m = \begin{cases} \frac{M-1}{2}, & M \text{ odd} \\ \frac{M}{2}, & M \text{ even,} \end{cases} \tag{48}$$

we write once more

$$f(z) = \prod_{i=1}^{2m} (z^2 - \varepsilon_i z + 1), \quad \varepsilon_i = z_i + z_i^{-1} \tag{49}$$

for the reduced polynomial. From the two alternative expressions for f we obtain a linear system of equations for the elementary symmetric polynomials $e_k = e_k(\varepsilon_1, \dots, \varepsilon_m)$ in the roots ε_i . Solving this system we then define the polynomial

$$F(\varepsilon) = \sum_{k=0}^{2m} (-1)^k e_k \varepsilon^{m-k} = \prod_{i=1}^m (\varepsilon - \varepsilon_i)(\varepsilon + \varepsilon_i).$$

We now explicitly state this polynomial F for $\alpha = -\beta$ on the imaginary axis. We have to distinguish the cases of odd and even sites:

$M = 2m + 1.$

$$F(\varepsilon) = (-)^m \sum_{k=0}^m \frac{(-)^k \varepsilon^{2k}}{(2k+1)!} \left[\frac{(m+1+k)!}{(m-k)!} - g^2 \frac{(m+k)!}{(m-1-k)!} \right] \quad (50)$$

$$= 2 \frac{\sin \left[(M+1) \arccos \frac{\varepsilon}{2} \right] + g^2 \sin \left[(M-1) \arccos \frac{\varepsilon}{2} \right]}{\varepsilon \sqrt{4 - \varepsilon^2}}. \quad (51)$$

$M = 2m.$

$$F(\varepsilon) = (-)^m \sum_{k=0}^m \frac{(-)^k \varepsilon^{2k}}{(2k)!} \left[\frac{(m+k)!}{(m-k)!} - g^2 \frac{(m-1+k)!}{(m-1-k)!} \right] \quad (52)$$

$$= 2 \frac{\sin \left[(M+1) \arccos \frac{\varepsilon}{2} \right] + g^2 \sin \left[(M-1) \arccos \frac{\varepsilon}{2} \right]}{\sqrt{4 - \varepsilon^2}}. \quad (53)$$

The expressions in terms of the inverse function arccos can be checked by rewriting the Bethe ansatz equations (39). At $\alpha = -\beta = ig$, the latter simplify to the transcendental equation

$$1 = z^{2M} \frac{\beta + z}{\beta + z^{-1}} \frac{1 + \alpha z^{-1}}{1 + \alpha z} = z^{2M} \frac{z^2 + g^2}{1 + z^2 g^2} \Leftrightarrow g^2 = -\frac{\sin[(M+1)\zeta]}{\sin[(M-1)\zeta]}, \quad z = \exp(i\zeta). \quad (54)$$

This is in agreement with the above expressions for the single-particle energies as zeros of (51) and (53). Note, however, that the polynomial expressions (50) and (52) are of advantage in the numerical computation of the single-particle energies. From (50) one also easily spots the occurrence of another zero mode $\varepsilon = 0$ at $g^2 = (M+1)/(M-1)$ for M odd which we will connect below with a representation of the universal enveloping algebra of the Lie superalgebra $\mathfrak{gl}(1|1)$. We will also exploit the above polynomials and their expressions in terms of inverse trigonometric functions to derive approximations for the single-particle energies in the interval $0 < g < 1$.

3.2. Groundstate eigenvalues and central charges

Using the results from the previous section we can expand the single-particle energies as power series in the coupling parameter g^2 . Employing the equation

$$F(\varepsilon) = 0$$

we find the following approximated expressions in the vicinity of the points $g^2 = 0$ and $g^2 = 1$ where the exact solutions are known:

$$0 < g \ll 1 : \varepsilon_k = 2 \cos \frac{\pi k}{M+1} - 2g^2 \frac{\sin \frac{\pi k}{M+1} \sin \frac{2\pi k}{M+1}}{M+1} + O(g^4), \quad k = 1, \dots, M \quad (55)$$

and

$$0 \ll g < 1 : \varepsilon_k = 2 \cos \frac{\pi k}{M} + (1 - g^2) \frac{\sin \frac{\pi k}{M} \tan \frac{\pi k}{M}}{M} + O((1 - g^2)^2), \quad k = 1, \dots, M - 1. \quad (56)$$

If M is even we have to omit the value $k = M/2$ where the above approximation is not valid since we then have a zero mode at $g = 1$ and the equation $F(0) = 0$ becomes trivial. For M even we thus approximate the two missing eigenvalues which converge to $\varepsilon = 0$ at $g = 1$ by

$$\varepsilon_{M/2}^\pm = \pm 2 \sqrt{\frac{2(1 - g^2)}{M(M+2 - g^2(M-2))}}.$$

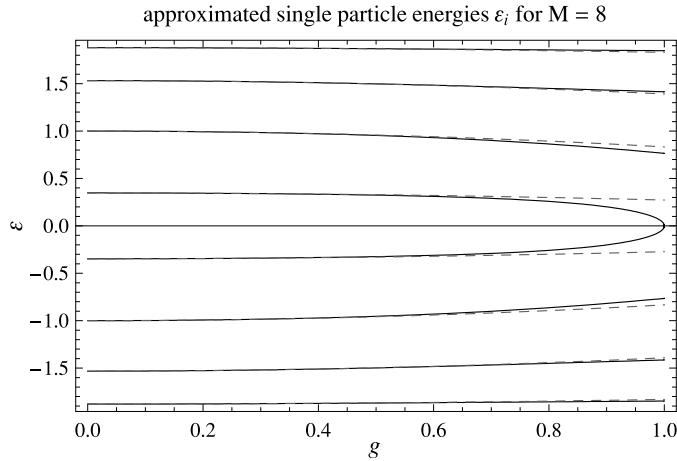


Figure 2. Approximations of the single-particle energies in the vicinity of $g = 0$.

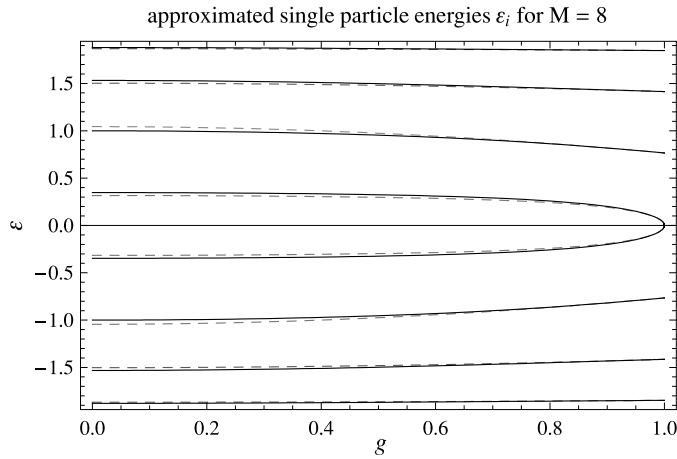


Figure 3. Approximations of the single-particle energies in the vicinity of $g = 1$.

This approximation is found by expanding the Bethe ansatz equations (53) at $\varepsilon = 0$. An example, $M = 8$, for these approximations is shown in figures 2 and 3. The solid lines indicate the exact single-particle energies ε_i and the dashed lines the approximations. In the vicinity of $g = 0$ the approximations are depicted in figure 2.

For the approximations in the vicinity of $g = 1$ see figure 3.

Having found approximated expressions for the single-particle energies ε_i , we can derive approximations for the groundstate eigenvalue E_0 of (7) and discuss the finite size corrections of the system as it approaches the two points $g = 0$ and $g = 1$. For the latter values the result is well known, see table 1.

Using these expansions in the system size M , one obtains via the general formula [35, 36]

$$E_0 = 2Mf_\infty + f_s - \frac{\pi c_{\text{eff}}}{12M} + O\left(\frac{1}{M^2}\right) \quad (57)$$

the effective central charge $c_{\text{eff}} = c - 12d_{\text{min}}$ of the conformal field theory describing the system in the thermodynamic limit. Here, d_{min} is the smallest scaling dimension occurring in

Table 1. Expansion of the groundstate energy with respect to the lattice size M .

	$g = 0$	$g = 1$
M odd	$E_0 = 1 - \frac{2(M+1)}{\pi} + \frac{\pi}{6M} + O\left(\frac{1}{M^2}\right)$	$E_0 = 1 - \frac{2M}{\pi} - \frac{\pi}{12M} + O\left(\frac{1}{M^2}\right)$
M even	$E_0 = 1 - \frac{2(M+1)}{\pi} - \frac{\pi}{12M} + O\left(\frac{1}{M^2}\right)$	$E_0 = 1 - \frac{2M}{\pi} + \frac{\pi}{6M} + O\left(\frac{1}{M^2}\right)$

the theory and f_∞ and f_s are the bulk and surface free energy, respectively. One recovers the familiar central charges at $g = 1$ mentioned in the introduction: for an odd number of sites the conformal anomaly is $c = 1$ ($d_{\min} = 0$), while it is $c = -2$ for M even ($d_{\min} = 0$). Note that for M odd at $g = 0$ we also formally obtain $c_{\text{eff}} = -2$, it appears however that this case has not been investigated further in the literature [37].

Let us now consider the approximate expressions for $0 < g < 1$. Summing the above expressions for the single-particle energies we arrive at

M odd, $0 < g \ll 1$:

$$\begin{aligned}
 E_0 &= -\sum_{k=1}^{\frac{M-1}{2}} \varepsilon_k = 1 - \frac{\cos \frac{\pi}{2(M+1)}}{\sin \frac{\pi}{2(M+1)}} + \frac{2 \cos \frac{\pi}{M+1} \cos \frac{\pi}{2(M+1)}}{(M+1) \sin \frac{3\pi}{2(M+1)}} g^2 + O(g^4) \\
 &= 1 + \frac{4g^2}{3\pi} - \frac{2(M+1)}{\pi} + \frac{\pi}{6M} + O(M^{-2}) + O(g^4). \tag{58}
 \end{aligned}$$

M even, $0 < g \ll 1$:

$$\begin{aligned}
 E_0 &= -\sum_{k=1}^{\frac{M}{2}} \varepsilon_k = 1 - \frac{1}{\sin \frac{\pi}{2(M+1)}} + \frac{1 + \cos \frac{\pi}{M+1}}{(M+1) \sin \frac{3\pi}{2(M+1)}} g^2 + O(g^4) \\
 &= 1 + \frac{4g^2}{3\pi} - \frac{2(M+1)}{\pi} - \frac{\pi}{12M} + O(M^{-2}) + O(g^4). \tag{59}
 \end{aligned}$$

Thus, in both cases, we only see a change in the surface term f_s up to order g^2 in the vicinity of $g = 0$. A computation of the second derivative $\varepsilon_k''(g^2 = 0)$ using the equation $F(\varepsilon) = 0$ shows that also the g^4 contribution to the groundstate only contributes to the surface energy. The computation of higher orders becomes cumbersome and it might be preferable to rely on field-theoretic methods instead, we briefly comment on this in the conclusions.

Let us now turn to the case when g is the vicinity of $g = 1$ to see whether we encounter a shift in the central charge here. Again we sum the approximate expressions of the single-particle energies to obtain the expression for the groundstate eigenvalue. Unlike for $g = 0$ we cannot find exact expressions at this point. Instead we split the sum over the correction terms for $g < 1$ into two parts,

$$\sum_k \frac{\sin \frac{\pi k}{M} \tan \frac{\pi k}{M}}{M} = \frac{1}{M} \sum_k \frac{1}{\cos \frac{\pi k}{M}} - \frac{1}{M} \sum_k \cos \frac{\pi k}{M},$$

and for $M > 4$ employ the Euler–Maclaurin formula to obtain the following approximations for the first sum:

$$M \text{ odd, } 0 \ll g < 1 : \frac{1}{M} \sum_{k=1}^{\frac{M-1}{2}} \frac{1}{\cos \frac{\pi k}{M}} \approx \frac{4 - 3 \ln \frac{1}{M} + 3 \ln \frac{4}{\pi}}{3\pi} - \frac{1}{2M} + O\left(\frac{1}{M^2}\right) \tag{60}$$

and

$$M \text{ even, } 0 \ll g < 1 : \frac{1}{M} \sum_{k=1}^{\frac{M}{2}-1} \frac{1}{\cos \frac{\pi k}{M}} \approx \frac{7 - 12 \ln \frac{1}{M} + 12 \ln \frac{2}{\pi}}{12\pi} - \frac{1}{2M} + O\left(\frac{1}{M^2}\right). \tag{61}$$

For M even we have another contribution from the energy level which becomes a zero mode at $g = 1$. Keeping $\delta = 1 - g^2$ fixed and choosing M large enough such that $\delta M \gg 1$ we find the asymptotic expansion

$$\varepsilon_{M/2} = \frac{2\sqrt{2}}{M} - \frac{2\sqrt{2}(2-\delta)}{\delta M^2} + O\left(\frac{1}{\delta^2 M^3}\right), \quad \delta := 1 - g^2. \quad (62)$$

However, for our purposes this is not a good approximation since it should vanish at $g = 1$. If we therefore expand first with respect to δ , we find instead

$$\varepsilon_{M/2} = \sqrt{\frac{2\delta}{M}} - \frac{(M-2)}{4\sqrt{2}M} \delta^{3/2} + O(\delta^{5/2}). \quad (63)$$

From this approximation we cannot infer the correct finite size scaling properties. In order to extract conclusive results about the finite size scaling behaviour, we therefore need to find the exact solutions for the single-particle energies first. For now we have to leave this problem open, but we hope to address it in future work by field-theoretic methods and exploiting the underlying algebraic structures which we highlight next.

4. Quasi-fermions and $U(\mathfrak{gl}(1|1))$ invariance

As we saw in the previous section the spectrum of the Hamiltonian is composed out of single-particle excitations with energies $\varepsilon_i = z_i + z_i^{-1}$ which are ‘created’ from a pseudo-vacuum applying the creation operator (36). Naturally, we wish to find the corresponding annihilation operator in order to set up a fermion or CAR algebra in quasi-momentum space which diagonalizes the Hamiltonian. As the Hamiltonian is non-Hermitian, the annihilation operator of momentum $k = -i \ln z$ cannot simply be the Hermitian adjoint of (36) with respect to the original inner product. Instead we introduce the time-reversed annihilation operator

$$\hat{d}_z := T \hat{c}_z T = \sum_{x=1}^M \psi_z(x; \alpha, \beta = \bar{\alpha}) c_x, \quad (64)$$

where the conjugation with the time-reversal operator is motivated by observing that

$$THT = H^* \quad \text{for} \quad \beta = \bar{\alpha}.$$

Obviously, we then obtain the desired commutation relation

$$[H, \hat{d}_z] = (z + z^{-1}) \hat{d}_z, \quad (65)$$

i.e. \hat{d}_z annihilates a quasi-particle of energy $\varepsilon = z + z^{-1}$.

Alternatively, we could also have employed the parity operator P in definition (64), since $PHP = H^*$. However, up to a phase factor this would lead to the same result due to the following identities of the wavefunction $\psi_z(x; \alpha) := \psi_z(x; \alpha, \beta = \bar{\alpha})$:

$$\psi_z(M+1-x; \alpha) = -z^{M+1} \frac{1 + \bar{\alpha}/z}{1 + \bar{\alpha}z} \psi_z(x; \bar{\alpha}) = -z^{M+1} \overline{\psi_z(x; \alpha)}. \quad (66)$$

Here we have assumed that z is a solution of (39) and hence, lies on the unit circle. From (66) together with (33) we infer that

$$PT \hat{c}_z^* PT = -z^{-M-1} \hat{c}_z^* \quad \text{and} \quad P \hat{c}_z P = -z^{-M-1} \hat{d}_z. \quad (67)$$

This, in particular, implies that the system possesses PT symmetry, i.e. the eigenstates of the Hamiltonian can be chosen to be eigenvectors of the PT operator. However, this fact does not guarantee quasi-Hermiticity which we show next.

Our strategy for establishing quasi-Hermiticity is to turn operators (36) and (64) into a well-defined representation of the fermionic oscillator or CAR algebra. Under an appropriate renormalization of wavefunction (37),

$$\psi_z(x; \alpha) \rightarrow \frac{a_z \psi_z(x; \alpha)}{(-2M a_z a_{z^{-1}} + [M]_z (z^{M+1} a_{z^{-1}}^2 + z^{-M-1} a_z^2))^{\frac{1}{2}}}, \quad a_z := 1 + \alpha/z, \quad (68)$$

one verifies that the following anticommutation relations hold:

$$[\hat{c}_{z_1}^*, \hat{c}_{z_2}^*]_+ = [\hat{d}_{z_1}, \hat{d}_{z_2}]_+ = 0 \quad \text{and} \quad [\hat{c}_{z_1}^*, \hat{d}_{z_2}]_+ = \delta_{z_1, z_2}. \quad (69)$$

Here, z_1, z_2 are two solutions to the Bethe ansatz equations (39). The anticommutation relations (32) are a direct consequence of the wavefunction identities

$$\sum_x \psi_{z_k}(x) \psi_{z_l}(x) = \delta_{kl} \quad \text{and} \quad \sum_k \psi_{z_k}(x) \psi_{z_k}(y) = \delta_{x,y}, \quad (70)$$

where the index k labels the solutions to the Bethe ansatz equations. Note that these identities lead to the inversion formulae

$$c_x^* = \sum_k \psi_{z_k}(x) \hat{c}_{z_k}^* = \sum_k \overline{\psi_{z_k}(x)} \hat{d}_{z_k}^* \quad (71)$$

and

$$c_x = \sum_k \overline{\psi_{z_k}(x)} \hat{c}_{z_k} = \sum_k \psi_{z_k}(x) \hat{d}_{z_k}. \quad (72)$$

While we have obtained the correct anticommutation relations in quasi-momentum space, the algebras generated by $\{\hat{c}_z^*, d_z\}$ do not possess the right $*$ -structure (anti-involution), where creation and annihilation operators are related by Hermitian conjugation. However, we now introduce the quasi-Hermiticity operator and the associated inner product with respect to which (36) and (64) possess the right $*$ -structure.

Theorem 2. *The Hamiltonians (1) and (2) are quasi-Hermitian for $\alpha = \bar{\beta}$ and $|\alpha| < 1$. Let $z_j = \exp(ik_j)$, $j = 1, \dots, M$, be the M roots of polynomial (44) not containing a reciprocal pair ($k_j \neq -k_{j'}$ for all j, j'), then*

$$H = -\frac{\alpha + \bar{\alpha}}{2} - \sum_{j=1}^M 2 \cos k_j \hat{c}_{k_j}^* \hat{d}_{k_j}. \quad (73)$$

A similar expression holds for (2). The quasi-Hermiticity operator $\eta : V^{\otimes M} \rightarrow V^{\otimes M}$ and its inverse are given by

$$\eta = \sum_{n=0}^M \sum_{k_{j_1} < \dots < k_{j_n}} \hat{d}_{k_{j_1}}^* \dots \hat{d}_{k_{j_n}}^* |0\rangle \langle 0| \hat{d}_{k_{j_n}} \dots \hat{d}_{k_{j_1}} \quad (74)$$

and

$$\eta^{-1} = \sum_{n=0}^M \sum_{k_{j_1} < \dots < k_{j_n}} \hat{c}_{k_{j_1}}^* \dots \hat{c}_{k_{j_n}}^* |0\rangle \langle 0| \hat{c}_{k_{j_n}} \dots \hat{c}_{k_{j_1}}. \quad (75)$$

Besides quasi-Hermiticity of the Hamiltonian the map η also induces the conventional $*$ -structure of free fermions in quasi-momentum space via the identities

$$\eta \hat{c}_k^* = \hat{d}_k^* \eta \quad \text{and} \quad \eta \hat{d}_k = \hat{c}_k \eta, \quad k = 1, \dots, M. \quad (76)$$

Proof. First, we note that the creation operators (36) evaluated at the solutions $z = z_i$ of equations (39) provide us with a basis in the state space, see (41). Due to the symmetry of

equations (39) under the replacement $z \rightarrow z^{-1}$, there are only M relevant distinct solutions, despite the fact that the polynomial order is $2M + 2$. According to the anticommutation relations (69) these solutions then yield $2^M = \dim V^{\otimes M}$ eigenvectors. The assertions then follow from the previous proposition showing that all Bethe roots lie on the unit circle for $\alpha = \bar{\beta}$ and $|\alpha| < 1$ as well as employing (40) and (69). \square

Corollary 3. *The C-operator $C = P\eta$ has the following expression in terms of creation and annihilation operators,*

$$C = \sum_{n=0}^M \sum_{k_{j_1} < \dots < k_{j_n}} (-1)^n e^{i(M+1)(k_{j_1} + \dots + k_{j_n})} \hat{c}_{k_{j_1}}^* \dots \hat{c}_{k_{j_n}}^* |0\rangle \langle 0| \hat{d}_{k_{j_n}} \dots \hat{d}_{k_{j_1}}. \quad (77)$$

Thus, with respect to the quasi-particle basis $\{|k_{j_1}, \dots, k_{j_n}\rangle = \hat{c}_{k_{j_1}}^* \dots \hat{c}_{k_{j_n}}^* |0\rangle\}_{n=0}^M$, the C-operator is simply given in terms of the total quasi-momentum operator $\hat{P} = \sum_r k_{j_r}$ and the quasi-particle number $\hat{N} = \sum_j \hat{c}_{k_j}^* \hat{d}_{k_j}$ as

$$C = (-1)^{\hat{N}} e^{i(M+1)\hat{P}}. \quad (78)$$

Proof. An immediate consequence from (67). \square

Let us summarize the result: the fermion or CAR algebra $\{c_x, c_x^*\}_{x=1}^M$ in position space with respect to the original inner product is replaced by a CAR algebra $\{\hat{d}_k, \hat{c}_k^*\}_{k=1}^M$ in quasi-momentum space with respect to the η -product,

$$\langle \hat{c}_k^* v, w \rangle_\eta = \langle v, \hat{c}_k \eta w \rangle = \langle v, \hat{d}_k w \rangle_\eta \quad (79)$$

and

$$\langle \hat{d}_k v, w \rangle_\eta = \langle v, \hat{d}_k^* \eta w \rangle = \langle v, \hat{c}_k^* w \rangle_\eta, \quad v, w \in V^{\otimes M}. \quad (80)$$

Note that there is another copy of this CAR algebra, namely $\{\hat{d}_k^*, \hat{c}_k\}_{k=1}^M$ but with respect to the η^{-1} -product.

We have excluded the unit circle from the allowed range of the boundary parameter α . While the spectrum of H is also real in this case, it does not necessarily imply the existence of a positive definite operator η , i.e. quasi-Hermiticity is a stronger condition. This is linked to the appearance of Jordan blocks in the Jordan normal form of the Hamiltonian as we will now discuss for the special case when $\alpha = -\beta = ig, g \geq 0$. Without loss of generality we can restrict ourselves to positive values of g , since g and $-g$ are related via spin reversal. We will show that the appearance of non-trivial Jordan blocks coincides with the vanishing of a central element in a representation of a specific superalgebra.

4.1. 'Deformed' quantum group symmetry on the imaginary axis

Since the Hamiltonians (1), (2) and (7) can be expressed in terms of free fermions as we have just seen, there are several symmetries and algebraic structures associated with them. These have been previously investigated for α, β on the unit circle. Here we shall show that these symmetries and algebras can be extended inside the unit disc along the imaginary axis setting $\alpha = -\beta = ig, g \geq 0$. We shall also relate the new inner product to the representations of these algebras. We start by reviewing the known symmetries and algebras for the case $g = 1$, i.e. α, β on the unit circle.

It is well known that for $g = 1$ the Hamiltonian (7) possesses a $U_q(sl_2)$ symmetry with $q = i \equiv \sqrt{-1}$ [5]. Below we shall see that for an odd number of sites, $M \in 2\mathbb{N} + 1$, this

symmetry can be extended along the imaginary axis for $0 \leq g < \sqrt{(M+1)/(M-1)}$. We also comment on a deformation of the Temperley–Lieb algebra [23, 24] (see [25] for a text book), which is the commutant of $U_q(sl_2)$. First, we recall the basic algebraic definitions.

Definition 1. *The q -deformed enveloping algebra $U_q(sl_2)$ is defined in terms of the Chevalley generators $\{E, F, K^{\pm 1}\}$ and the relations*

$$K K^{-1} = K^{-1} K = 1, \quad K E = q^2 E K, \quad K F = q^{-2} F K, \quad [E, F] = \frac{K - K^{-1}}{q - q^{-1}}. \tag{81}$$

Definition 2. *The Temperley–Lieb algebra $TL_M(q)$ is the associative, unital algebra generated by $\{e_i\}_{i=1}^{M-1}$ subject to the identities*

$$e_i^2 = -(q + q^{-1})e_i, \quad e_i e_{i\pm 1} e_i = e_i, \quad e_i e_j = e_j e_i, \quad |i - j| > 1. \tag{82}$$

Setting the deformation parameter to $q = \sqrt{-1}$ we obtain at $g = 1$ the following representations of the two algebras

$$K^{\pm 1} \mapsto i^{\pm M} \prod_{x=1}^M \sigma_x^z, \quad E \mapsto \sum_x i^{x-1} c_x^*, \quad F \mapsto \sum_x i^x c_x K^{-1} \tag{83}$$

and

$$e_x \mapsto c_x c_{x+1}^* - c_x^* c_{x+1} + i(n_x - n_{x+1}), \quad x = 1, 2, \dots, M - 1. \tag{84}$$

One easily verifies that the above algebraic relation of $U_q(sl_2)$ and $TL_M(q)$ is satisfied. In addition, we have the identities

$$E^2 = F^2 = 0 \quad \text{and} \quad K^2 = (-1)^M. \tag{85}$$

Moreover, we have that the action of the Temperley–Lieb and the quantum algebra commute (this is a special case of the quantum analogue of Schur–Weyl duality [27]),

$$[U_q(sl_2), TL_M(q)] = 0, \tag{86}$$

whence the Hamiltonian

$$g = 1 : \quad H = H' = \sum_{x=1}^{M-1} e_x \tag{87}$$

is quantum group invariant. For $g = 1$ these relations hold for both, odd and even numbers of sites. However, note that we have

$$[E, F] = \begin{cases} 0, & M \text{ even} \\ i^{M-1} K, & M \text{ odd.} \end{cases} \tag{88}$$

As we shall see below, the vanishing of the commutator for M even is closely related to the fact that the discrete wavefunction of an associated fermionic zero mode has vanishing norm,

$$\sum_x \psi_{k=i}(x)^2 = 0.$$

This has profound consequences for the quasi-Hermiticity of the Hamiltonian, since the quasi-Hermiticity operator η ceases to be positive *definite*, $\eta > 0$, and instead becomes positive *semi-definite*, $\eta \geq 0$. One of the novel results in this paper is the observation that a similar scenario also happens for M odd, albeit at the value $g = \sqrt{\frac{M+1}{M-1}} > 1$. In order to discuss these

issues and to interpret the new inner product in terms of representation theory it is favourable to introduce yet another algebra.

Definition 3. *The universal enveloping algebra $U(\mathfrak{gl}(1|1))$ of the superalgebra $\mathfrak{gl}(1|1)$ is the \mathbb{Z}_2 -graded associative algebra (over \mathbb{C}) generated by the odd (fermionic) elements $\{X^\pm\}$ and the even (bosonic) elements $\{Y, Z\}$ satisfying the relations*

$$[Y, X^\pm] = \pm X^\pm, \quad [Z, Y] = [Z, X^\pm] = 0, \quad [X^+, X^-]_+ = Z. \quad (89)$$

There is a natural anti-involution or $*$ -structure on $U(\mathfrak{gl}(1|1))$ by setting

$$(X^\pm)^* = X^\mp, \quad Y^* = Y, \quad Z^* = Z. \quad (90)$$

The following $U(\mathfrak{gl}(1|1))$ -representation at $g = 1$ is a special case of the representation discussed in [13] for the deformed case $U_q(\mathfrak{gl}(1|1))$ on which we will comment later,

$$X^+ \mapsto \sum_x i^{x-1} c_x^*, \quad X^- \mapsto \sum_x i^{x-1} c_x, \quad Y \mapsto S^z, \quad Z \mapsto \begin{cases} 0, & M \text{ even} \\ M\mathbf{1}, & M \text{ odd.} \end{cases} \quad (91)$$

Again, we observe a crucial difference for the two cases M even and odd: the vanishing of the central element Z . We will now discuss for $g \neq 1$ an extension of the above representation. For M even we shall see that (91) is a singular limit of a representation with $Z \neq 0$. However, we start our discussion with the case M odd, since it is more well behaved and shall then move on to M even pointing out similarities and differences for $0 \leq g \leq 1$.

4.2. Odd number of sites

For M odd the quantum group symmetry can be extended. As noted earlier we have for $\theta = \pi/2$ and M odd the following two Bethe roots $z_1 = \pm\sqrt{-1}$ giving rise to a zero mode of the Hamiltonian (we shall focus on $z = i$):

$$[H, \hat{c}_{z=i}^*] = [H, \hat{d}_{z=i}] = 0, \quad (92)$$

where the corresponding wavefunction is given by

$$\psi_{z=i}(x) = \frac{\sin \frac{\pi x}{2} - ig \cos \frac{\pi x}{2}}{\sqrt{\frac{M+1}{2} - \frac{M-1}{2} g^2}}. \quad (93)$$

This solution prompts the following operator definitions:

$$U = \sum_x \sin \frac{\pi x}{2} c_x = \sum_{x \text{ odd}} (-1)^{\frac{x-1}{2}} c_x \quad (94)$$

and

$$V = \sum_x \cos \frac{\pi x}{2} c_x = \sum_{x \text{ even}} (-1)^{\frac{x}{2}} c_x, \quad (95)$$

such that

$$\hat{c}_{z=i}^* = \frac{U^* - igV^*}{\sqrt{\frac{M+1}{2} - \frac{M-1}{2} g^2}} \quad \text{and} \quad \hat{d}_{z=i} = \frac{U - igV}{\sqrt{\frac{M+1}{2} - \frac{M-1}{2} g^2}}. \quad (96)$$

The operators U and V satisfy the relations

$$U^2 = V^2 = [U, V]_+ = [U, V^*]_+ = [U^*, V]_+ = 0 \quad (97)$$

and

$$[U, U^*]_+ = \frac{M+1}{2} \mathbf{1}, \quad [V, V^*]_+ = \frac{M-1}{2} \mathbf{1}. \quad (98)$$

Thus, up to a trivial renormalization, $U \rightarrow U/\sqrt{(M+1)/2}$ and $V \rightarrow V/\sqrt{(M-1)/2}$, we can think of U and V as two fermionic oscillators. Alternatively, we can also interpret them as two representations of the *non-deformed* superalgebra $\mathfrak{gl}(1|1)$ introduced above by identifying

$$Y \mapsto S^z, \quad Z \mapsto \frac{M+1}{2}\mathbf{1}, \quad X^+ \mapsto U^*, \quad X^- \mapsto U \quad (99)$$

and

$$Y \mapsto S^z, \quad Z \mapsto \frac{M-1}{2}\mathbf{1}, \quad X^+ \mapsto V^*, \quad X^- \mapsto V. \quad (100)$$

We thus obtain two distinct representations of $\mathfrak{gl}(1|1)$ which, in addition, preserve the $*$ -structure (90) with respect to the original inner product. For $0 < g < 1$, neither of these two representations by itself give rise to a symmetry of the Hamiltonian, instead we have to consider the combined representation

$$\begin{aligned} Y &\mapsto S^z, & Z &\mapsto \left(\frac{M+1}{2} - g^2 \frac{M-1}{2} \right) \mathbf{1}, \\ X^+ &\mapsto U^* - igV^*, \\ X^- &\mapsto U - igV. \end{aligned} \quad (101)$$

According to (92) the generators X^\pm create, respectively, annihilate zero modes of the Hamiltonian and we therefore have an $U(\mathfrak{gl}(1|1))$ symmetry of the Hamiltonian (7),

$$[H_g, U(\mathfrak{gl}(1|1))] = 0, \quad 0 \leq g < \sqrt{\frac{M+1}{M-1}}. \quad (102)$$

Note that in representation (101) the $*$ -structure (90) is not preserved with respect to the original inner product,

$$X^\pm \neq (X^\mp)^*, \quad (103)$$

but with respect to the new inner product induced by η ,

$$\eta X^\pm = (X^\mp)^* \eta. \quad (104)$$

This allows one to interpret the new Hilbert space structure induced by η in a purely representation theoretic setting. It also singles out the $U(\mathfrak{gl}(1|1))$ symmetry over the $U_q(\mathfrak{sl}_2)$ symmetry whose extension we discuss next.

Namely, for $M \in 2\mathbb{N} + 1$, $0 \leq g < \sqrt{\frac{M+1}{M-1}}$ and $q = \sqrt{-1}$, we now set

$$K^{\pm 1} \mapsto i^{\pm M} \prod_{x=1}^M \sigma_x^z, \quad E \mapsto \frac{U^* - igV^*}{\sqrt{\frac{M+1}{2} - \frac{M-1}{2}g^2}}, \quad F \mapsto \frac{-(gV + iU)K}{\sqrt{\frac{M+1}{2} - \frac{M-1}{2}g^2}}. \quad (105)$$

Employing the anticommutation relations for U and V and their Hermitian adjoints, one easily verifies that this representation is well defined and that relations (85) continue to hold. Apparently, we recover the familiar representation (83) on the unit circle in the limit $g \rightarrow 1$.

The obvious guess for an extension of the Temperley–Lieb algebra for $g \geq 0$,

$$e_x \mapsto c_x c_{x+1}^* - c_x^* c_{x+1} + ig(n_x - n_{x+1}), \quad x = 1, 2, \dots, M-1, \quad (106)$$

does yield the modified commutation relations

$$e_x^2 = (1 - g^2)[(1 - n_x)n_{x+1} + n_x(1 - n_{x+1})] \quad (107)$$

and

$$e_x e_{x\pm 1} e_x = g^2 e_x + ig(1 - g^2)(n_x - n_{x+1})[1 + (n_{x\pm 1} - n_{x\pm 1\pm 1})(n_x - n_{x+1})]. \quad (108)$$

This extension of the Temperley–Lieb algebra in terms of ‘local Hamiltonians’, i.e. the nearest-neighbour terms, does not preserve the algebraic structure at $g = 1$. Furthermore, Schur–Weyl duality is broken for $g < 1$: the commutation relations between the fermionic oscillators and the extended Temperley–Lieb generators (106) are

$$[U, e_x] = \begin{cases} (-)^{\frac{x+1}{2}} (c_{x+1} - igc_x), & x \text{ odd} \\ (-)^{\frac{x+2}{2}} (c_x + igc_{x+1}), & x \text{ even}, \end{cases} \tag{109}$$

$$[V, e_x] = \begin{cases} (-)^{\frac{x-1}{2}} (c_x + igc_{x+1}), & x \text{ odd} \\ (-)^{\frac{x+2}{2}} (c_{x+1} - igc_x), & x \text{ even}, \end{cases} \tag{110}$$

whence we now have for the quantum group generators the identities

$$0 \leq g \leq \sqrt{\frac{M+1}{M-1}} : [E, e_x + e_{x+1}] = [F, e_x + e_{x+1}] = 0, \quad x = 1, 3, 5, \dots, M-2. \tag{111}$$

Thus, while for $M \in 2\mathbb{N} + 1$ the Hamiltonian remains quantum group invariant for all values $0 \leq g \leq \sqrt{\frac{M+1}{M-1}}$, we now have to consider pairs of the extended Temperley–Lieb generators.

Note that representation (105) becomes singular at $g^2 = (M+1)/(M-1)$, this is also the value where the fermionic modes $X^+ = U^* - igV^*$ and $X^- = U - igV$ anticommute,

$$g^2 = \frac{M+1}{M-1} : [X^+, X^-]_+ = Z = 0. \tag{112}$$

This is precisely the scenario mentioned above for M even at $g = 1$. We see that the associated wavefunction (93) becomes singular as its norm vanishes. Moreover, the Jordan normal form J of the Hamiltonian now possesses non-trivial 3×3 blocks. For instance, we have for $M = 5$ and the sector $S^z = 1/2$ the Jordan normal form,

$$J = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \dots & \dots & 0 \\ 0 & 0 & 1 & 0 & 0 & & & \vdots \\ \vdots & 0 & 0 & 1 & 0 & & & \\ & \vdots & 0 & 0 & 0 & 0 & & \\ & & \vdots & 0 & -\sqrt{\frac{5}{2}} & 1 & 0 & \\ & & & \vdots & 0 & -\sqrt{\frac{5}{2}} & 1 & 0 & \vdots \\ & & & & \vdots & 0 & -\sqrt{\frac{5}{2}} & 0 & 0 & 0 \\ & & & & & \vdots & 0 & \sqrt{\frac{5}{2}} & 1 & 0 \\ \vdots & & & & & & 0 & 0 & \sqrt{\frac{5}{2}} & 1 \\ 0 & \dots & & & & & 0 & 0 & 0 & \sqrt{\frac{5}{2}} \end{pmatrix}.$$

Some of the eigenvalues smoothly join up as can be seen in figure 4.

Beyond the threshold value $g^2 = \frac{M+1}{M-1}$ the Hamiltonian has complex eigenvalues. Thus, quasi-Hermiticity of the Hamiltonian can only hold for $g^2 < \frac{M+1}{M-1}$ and this value approaches the unit circle as $M \rightarrow \infty$.

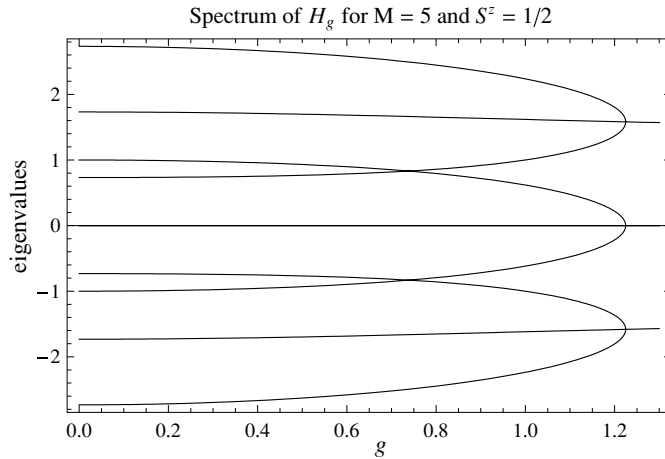


Figure 4. Spectrum of the Hamiltonian (7).

4.3. Even number of sites

For M even we define the operators U and V analogously to (94) and (95), and obtain again representations of $\mathfrak{gl}(1|1)$. But we now have

$$[U, U^*]_+ = [V, V^*]_+ = \frac{M}{2} \mathbf{1} \quad \text{and} \quad Z \mapsto \frac{M}{2} (1 - g^2) \mathbf{1}. \quad (113)$$

The definition of the other operators in (101) is unchanged. Due to the absence of a zero mode, we do not obtain as before a $U(\mathfrak{gl}(1|1))$ symmetry of the *full* Hamiltonian. Instead the generators X^\pm only commute with the *truncated* Hamiltonian where the last Temperley–Lieb generator is omitted,

$$[H_g^{\text{trunc}}, U(\mathfrak{gl}(1|1))] = 0 \quad (114)$$

with

$$H_g^{\text{trunc}} = H_g - e_{M-1} = \sum_{x=1}^{M-2} e_x = \frac{1}{2} \sum_{x=1}^{M-2} [\sigma_m^x \sigma_{m+1}^x + \sigma_m^y \sigma_{m+1}^y + ig(\sigma_m^z - \sigma_{m+1}^z)]. \quad (115)$$

This already signals that this representation mimics the one of the chains with $M - 1$ sites. There is more evidence for this interpretation: for an extension of the $U_q(\mathfrak{sl}_2)$ representation one now needs to introduce the operators

$$M \in 2\mathbb{N} : \quad K^{\pm 1} = i^{\pm M \mp 1} \prod_{x=1}^M \sigma_x^z, \quad E = \frac{U^* - igV^*}{\sqrt{\frac{M}{2}(1 - g^2)}}, \quad F = -\frac{(gV + iU)K}{\sqrt{\frac{M}{2}(1 - g^2)}}, \quad (116)$$

which again satisfy the right commutation relations when setting $q = \sqrt{-1}$. Note, however, that the limit $g \rightarrow 1$ is now ill defined and that we have replaced $M \rightarrow M - 1$ in the Cartan generator K . As for M odd we have the relations

$$0 \leq g \leq 1 : \quad [E, e_x + e_{x+1}] = [F, e_x + e_{x+1}] = 0, \quad x = 1, 3, 5, \dots, M - 3. \quad (117)$$

An alternative way to restore quantum group or $U(\mathfrak{gl}(1|1))$ symmetry is by adding for $M/2$ even the generator

$$e_M = c_M c_1^* - c_M^* c_1 + ig(n_M - n_1) \quad (118)$$

and consider the Hamiltonian with periodic boundary conditions

$$H_{\text{periodic}} = \sum_{x=1}^M e_x = \sum_{x=1}^M (c_x c_{x+1}^* - c_x^* c_{x+1}), \quad M+1 \equiv 1. \quad (119)$$

The latter apparently does not depend on g and is simply the Hermitian Hamiltonian which describes free fermions on a lattice. We will not discuss this Hamiltonian further in the present context.

Finally, for M even there is an alternative representation of the quantum group symmetry which is obtained from PT reversal. Noting the transformation identities

$$PUP = \begin{cases} (-)^{\frac{M-1}{2}} U, & M \text{ odd} \\ (-)^{\frac{M}{2}} V, & M \text{ even} \end{cases} \quad \text{and} \quad PVP = \begin{cases} (-)^{\frac{M-1}{2}} V, & M \text{ odd} \\ (-)^{\frac{M}{2}} U, & M \text{ even} \end{cases} \quad (120)$$

one easily verifies that

$$K^{\pm 1} \mapsto i^{\mp M \pm 1} \prod_{x=1}^M \sigma_x^z, \quad E \mapsto \frac{V^* + igU^*}{\sqrt{\frac{M}{2}(1-g^2)}}, \quad F \mapsto -\frac{(gU - iV)K}{\sqrt{\frac{M}{2}(1-g^2)}} \quad (121)$$

yields another representation of $U_q(sl_2)$ with $q = -\sqrt{-1}$. The commutation relations (117) are then modified accordingly by conjugation with the PT operator.

Let us return to the case $g = 1$ for an even number of sites. If we only consider the fermionic oscillator modes X^\pm as before for M odd, then we see that they anticommute at $g = 1$, i.e. we have again $Z = 0$. We encounter the same scenario as before for M odd, the corresponding discrete wavefunction has zero norm,

$$M \in 2\mathbb{N} : \quad \sum_{x=1}^M \psi_{k=i}^2(x) = 0,$$

and the Hamiltonian has non-trivial Jordan blocks, however these are now of size 2×2 . To be concrete we state here the Jordan normal form J of the Hamiltonian for $M = 4$ when restricted to the $S^z = 0$ subspace,

$$J|_{S^z=0} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\sqrt{2} & 1 & 0 & 0 \\ 0 & 0 & 0 & -\sqrt{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \sqrt{2} & 1 \\ 0 & 0 & 0 & 0 & 0 & \sqrt{2} \end{pmatrix}.$$

Looking at the spectrum of the Hamiltonian we see once more that some eigenvalues smoothly join up at $g = 1$, as compared with figure 5.

This signals the appearance of complex eigenvalues for $|g| > 1$. Thus, quasi-Hermiticity only holds true inside the unit disc for M even.

5. Perturbation theory on the imaginary axis

While we have shown the existence of the map η for boundary fields $\alpha = \bar{\beta}$ inside the unit disc, its expression in terms of projectors on quasi-fermion states does not allow us to easily compute the corresponding Hermitian Hamiltonian

$$h = \eta^{1/2} H \eta^{-1/2}.$$

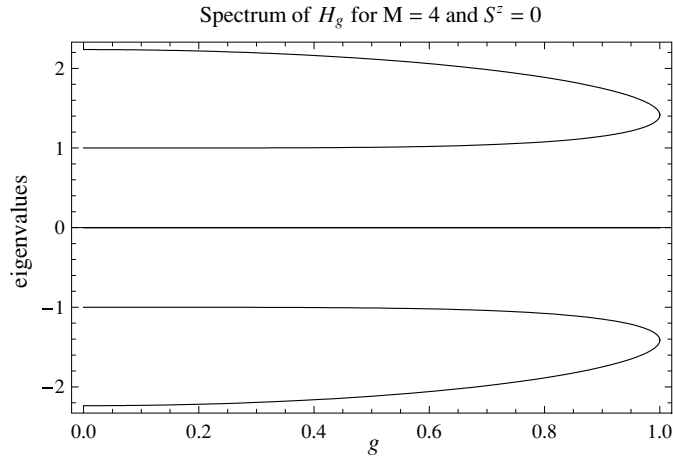


Figure 5. Spectrum of the Hamiltonian (7).

We now, therefore, specialize to the case $0 \leq g < 1$ and $\theta = \pi/2$ in (43) and compute it perturbatively. We will arrive at the result already presented in the introduction: the presence of non-Hermitian boundary terms leads to a long-range interaction in the bulk.

Since $\eta > 0$ we can write it in exponential form $\eta = \exp A$. The quasi-Hermiticity relation then translates into

$$H^* = e^A H e^{-A}. \tag{122}$$

Employing the Baker–Campbell–Hausdorff formula, the above identity can be expanded into multiple commutators

$$H + \sum_{k>0} \frac{1}{k!} \text{ad}_A^k H = H^*, \quad \text{ad}_X Y = [X, Y], \quad \eta = e^A. \tag{123}$$

This allows us to determine the operator A perturbatively by separating the non-Hermitian Hamiltonian H into an Hermitian and non-Hermitian part of the following form:

$$H = H_0 + igH_1, \quad H_0 = H_0^*, \quad H_1 = H_1^*, \quad 0 \leq g \ll 1. \tag{124}$$

The Hamiltonian (7) has precisely this structure. Setting the boundary parameters in (1) to purely imaginary values, $\alpha = -\beta = ig, g \in \mathbb{R}_+$, we define

$$H_0 = - \sum_{x=1}^{M-1} [c_x^* c_{x+1} - c_x c_{x+1}^*], \quad H_1 = \frac{\sigma_1^z - \sigma_M^z}{2} = n_1 - n_M. \tag{125}$$

Since we have $H_g^* = H_{-g}$ we demand $\eta_{-g} = \eta_g^{-1}$ leading to the following ansatz for a power series expansion of the metric operator in the coupling constant g :

$$A = \sum_{n \geq 0} g^{2n+1} A_{2n+1}. \tag{126}$$

From our previous considerations related to the appearance of Jordan blocks when the central element $Z \in \mathfrak{gl}(1|1)$ vanishes, we infer that the region of convergence for the above series is $0 \leq g < 1$ for M even and $0 \leq g < \sqrt{(M+1)/(M-1)}$ for M odd.

Theorem 4. *Collecting terms order by order in g we obtain the following equations for the coefficients in the expansion of the operator A :*

$$[H_0, A_1] = 2iH_1 \tag{127}$$

and for $n \geq 1$

$$[H_0, A_{2n+1}] = i \sum_{k=1}^n \lambda_k \sum_{p_1+\dots+p_{2k}=2n} [A_{p_1}, \dots, [A_{p_{2k}}, H_1] \dots]. \tag{128}$$

Here the sum runs over all compositions $p = (p_1, \dots, p_{2k})$ of $2n$ with $A_{p_i} = 0$ if p_i is even. The coefficients λ_k are determined recursively via

$$\lambda_1 = 1/6 \quad \text{and} \quad \lambda_k = \frac{2k-1}{(2k+1)!} - \sum_{j=1}^{k-1} \frac{\lambda_{k-j}}{(2j+1)!}, \quad k > 1. \tag{129}$$

The first elements in this sequence are

$$\lambda = \left(\frac{1}{6}, -\frac{1}{360}, \frac{1}{15\,120}, -\frac{1}{604\,800}, \frac{1}{23\,950\,080}, -\frac{691}{653\,837\,184\,000}, \frac{1}{37\,362\,124\,800}, \dots \right).$$

Proof. The recursion formula for the coefficients λ_k is proved via induction as follows. The case $n = 1$ is easily verified. Now assume that (128) holds true for all orders $k = 1, 2, \dots, n$. From the Baker–Campbell–Hausdorff formula

$$-2iH_1 = \sum_{k>0} \frac{1}{k!} \text{ad}_A^k H$$

we find that

$$\begin{aligned} [H_0, A_{2n+3}] &= i \sum_{k=1}^{n+1} \frac{1}{(2k)!} \sum_{p_1+\dots+p_{2k}=2n+2} [A_{p_1}, \dots, [A_{p_{2k}}, H_1] \dots] \\ &+ \sum_{k=1}^{n+1} \frac{1}{(2k+1)!} \sum_{p_1+\dots+p_{2k+1}=2n+3} [A_{p_1}, \dots, [A_{p_{2k+1}}, H_0] \dots]. \end{aligned}$$

Employing our assumption we can rewrite the second term on the right-hand side in terms of H_1 . For $p_{2k+1} = 1$ we find

$$[A_{p_{2k+1}}, H_0] = -2iH_1$$

and for $1 < p_{2k+1} \leq 2(n+1-k) + 1$ we have

$$[A_{p_{2k+1}}, H_0] = -i \sum_{j=1}^{\frac{p_{2k+1}-1}{2}} \lambda_j \sum_{q_1+\dots+q_{2j}=p_{2k+1}-1} [A_{q_1}, \dots, [A_{q_{2j}}, H_1] \dots].$$

Inserting these expressions, rearranging sums and collecting terms we find

$$\begin{aligned} [H_0, A_{2n+3}] &= i \sum_{k=1}^{n+1} \left\{ \frac{1}{(2k)!} - \frac{2}{(2k+1)!} - \sum_{j=1}^{k-1} \frac{\lambda_{k-j}}{(2j+1)!} \right\} \\ &\times \sum_{p_1+\dots+p_{2k}=2n+2} [A_{p_1}, \dots, [A_{p_{2k}}, H_1] \dots] \end{aligned}$$

which yields the desired recursion formula for the coefficients. □

In order to facilitate the comparison with results in the literature, we explicitly state the identities up to the order seven:

$$\begin{aligned}
 [H_0, A_1] &= 2iH_1, \\
 [H_0, A_3] &= \frac{i}{6}[A_1, [A_1, H_1]], \\
 [H_0, A_5] &= \frac{i}{6}[A_1, [A_3, H_1]] + \frac{i}{6}[A_3, [A_1, H_1]] - \frac{i}{360}[A_1, [A_1, [A_1, [A_1, H_1]]]]
 \end{aligned} \tag{130}$$

and

$$\begin{aligned}
 [H_0, A_7] &= \frac{i}{6}[A_3, [A_3, H_1]] + \frac{i}{6}[A_1, [A_5, H_1]] + \frac{i}{6}[A_5, [A_1, H_1]] \\
 &\quad - \frac{i}{360} \sum_{p_1+p_2+p_3+p_4=6} [A_{p_1}, [A_{p_2}, [A_{p_3}, [A_{p_4}, H_1]]]] \\
 &\quad + \frac{i}{15120}[A_1, [A_1, [A_1, [A_1, [A_1, [A_1, H_1]]]]]].
 \end{aligned}$$

Note that our general formula differs from equation (3.20) in [19] but reproduces the identities in equation (34) of [18].

One can now use identities (128) to compute the metric operator A order by order. In addition to the latter equations one also easily deduces from the properties η ought to obey that we must have

$$[A, S^z] = 0, \quad PA = -AP \quad \text{and} \quad A^* = A. \tag{131}$$

Define

$$a_{x,y}^\pm = c_x^* c_y \pm c_x c_y^*, \quad x < y \tag{132}$$

then we find that up to order 11 the terms in the expansion of the matrix A are of the general form

$$A_{2n+1} = \frac{(-1)^n i}{(2n+1)} \sum_{x=1}^{M-2n-1} a_{x,x+2n+1}^+ + \sum_{p=0}^{n-1} \sum_{x=1}^{n-p} i k_x^{(n,p)} (a_{x,x+2p+1}^+ + a_{M-x-2p,M+1-x}^+). \tag{133}$$

Explicitly, they read

$$\begin{aligned}
 A_1 &= i \sum_{x=1}^{M-1} a_{x,x+1}^+, \\
 A_3 &= \frac{1}{3i} \sum_{x=1}^{M-3} a_{x,x+3}^+ - \frac{1}{6i} (a_{1,2}^+ + a_{M-1,M}^+), \\
 A_5 &= \frac{i}{5} \sum_{x=1}^{M-5} a_{x,x+5}^+ + \frac{i}{24} (a_{1,2}^+ + a_{M-1,M}^+) + \frac{i}{120} (a_{2,3}^+ + a_{M-2,M-1}^+) - \frac{11i}{120} (a_{1,4}^+ + a_{M-3,M}^+), \\
 A_7 &= \frac{1}{7i} \sum_{x=1}^{M-7} a_{x,x+7}^+ - \frac{7}{240i} (a_{1,2}^+ + a_{M-1,M}^+) - \frac{1}{48i} (a_{2,3}^+ + a_{M-2,M-1}^+) \\
 &\quad - \frac{13}{840i} (a_{3,4}^+ + a_{M-3,M-2}^+) + \frac{1}{60i} (a_{1,4}^+ + a_{M-3,M}^+) \\
 &\quad - \frac{3}{560i} (a_{2,5}^+ + a_{M-4,M-1}^+) - \frac{103}{1680i} (a_{1,6}^+ + a_{M-5,M}^+)
 \end{aligned}$$

and

$$\begin{aligned}
 A_9 = & \frac{i}{9} \sum_{x=1}^{M-9} a_{x,x+9}^- + \frac{i}{64} (a_{1,2}^- + a_{M-1,M}^-) + \frac{23i}{2240} (a_{2,3}^- + a_{M-2,M-1}^-) \\
 & + \frac{17i}{1920} (a_{3,4}^- + a_{M-3,M-2}^-) + \frac{25i}{8064} (a_{4,5}^- + a_{M-4,M-3}^-) + \frac{11}{560i} (a_{1,4}^- + a_{M-3,M}^-) \\
 & + \frac{29}{1920i} (a_{2,5}^- + a_{M-4,M-1}^-) + \frac{587}{40\,320i} (a_{3,6}^- + a_{M-5,M-2}^-) \\
 & + \frac{113i}{13\,440} (a_{1,6}^- + a_{M-5,M}^-) + \frac{59}{8064i} (a_{2,7}^- + a_{M-6,M-1}^-) + \frac{1823}{40\,320i} (a_{1,8}^- + a_{M-7,M}^-).
 \end{aligned}$$

The stated solutions can be checked by employing the relations

$$\begin{aligned}
 [H_0, a_{x,y}^\pm] &= a_{x,y+1}^\mp - a_{x-1,y}^\mp + a_{x,y-1}^\mp - a_{x+1,y}^\mp, \\
 [H_1, a_{x,y}^\pm] &= (\delta_{x,1} + \delta_{y,M}) a_{x,y}^\mp, \quad x < y
 \end{aligned}$$

and

$$[a_{x,y}^+, a_{r,s}^-] = \delta_{y,r} a_{x,s}^- + \delta_{y,s} a_{x,r}^- - \delta_{x,s} a_{r,y}^- - \delta_{x,r} a_{s,y}^-.$$

Note that some of the terms in the general formula (133) vanish if $2n + 1 > M$. The general solution still needs to be found. Once the metric operator A is obtained, the corresponding Hermitian Hamiltonian h can be computed order by order. Define the Hermitian Hamiltonian h according to

$$h = e^{\frac{A}{2}} H e^{-\frac{A}{2}} = H_0 + \sum_{n=1}^{\infty} g^{2n} h_{2n}, \tag{134}$$

where the same region of convergence is implied as in the case of A .

Theorem 5. *The terms in the series expansion of h are given by*

$$h_{2n} = i \sum_{k=1}^n \lambda'_k \sum_{p_1+\dots+p_{2k-1}=2n-1} [A_{p_1}, \dots, [A_{p_k}, H_1] \dots], \tag{135}$$

where the sum runs over all compositions $p = (p_1, \dots, p_{2k-1})$ of $2n - 1$ and the coefficients λ'_k are computed from the coefficients λ_k in (128) via the formula

$$\lambda'_k = \frac{2k - 1}{2^{2k-1} (2k)!} - \sum_{j=1}^{k-1} \frac{\lambda_{k-j}}{2^{2j} (2j)!}. \tag{136}$$

The first terms in the above sequence are

$$\lambda' = \left(\frac{1}{4}, -\frac{1}{192}, \frac{1}{7680}, -\frac{17}{5160\,960}, \frac{31}{371\,589\,120}, -\frac{691}{326\,998\,425\,600}, \dots \right)$$

Proof. An induction proof similar to the previous one for the series expansion of the operator A . □

Again, we state the first terms explicitly in order to allow for comparison with the literature (see equation (3.24) in [19]),

$$\begin{aligned} h_2 &= \frac{i}{4}[A_1, H_1], \\ h_4 &= \frac{i}{4}[A_3, H_1] - \frac{i}{192}[A_1, [A_1, [A_1, H_1]]], \\ h_6 &= \frac{i}{4}[A_5, H_1] + \frac{i}{192} \sum_{p_1+p_2+p_3=5} [A_{p_1}, [A_{p_2}, [A_{p_3}, H_1]]] \\ &\quad + \frac{i}{7680}[A_1, [A_1, [A_1, [A_1, [A_1, H_1]]]]]. \end{aligned}$$

Note that h only depends on g^2 as it must due to $H_g^* = H_{-g}$. Inserting the explicit expressions for the series expansion of A up to order $n = 5$, we find the Hamiltonian stated in the introduction.

6. Exact results for short spin-chains

In this section, we present exact expressions for the quasi-Hermiticity operator η and the operator A employing the fact that for small M there are only a few terms appearing in the expressions for the operator A , as compared with (133). That is, motivated by our perturbation theory results we make the ansatz

$$A = \sum_{p=0}^{\lfloor M/2-1 \rfloor} \sum_{x=1}^{M-2p-1} \kappa_x^{(p)} (a_{x,x+2p+1}^+ + a_{M-x-2p,M+1-x}^+). \tag{137}$$

For M small enough one can exponentiate the resulting matrix and solve the intertwining relation in order to determine the coefficients $\kappa_x^{(p)}$. From our perturbative computation we can also make an educated guess about the form of the Hermitian Hamiltonian h in order to facilitate the computation of the similarity transformation. Namely, we make the ansatz

$$h = \sum_{p=0}^{\lfloor M/2-1 \rfloor} \sum_{x=1}^{M-2p-1} \xi_x^{(p)} (a_{x,x+2p+1}^- + a_{M-x-2p,M+1-x}^-). \tag{138}$$

Here we have used that h is parity invariant. This follows from the identities

$$P\eta^{\frac{1}{2}} = P e^{A/2} = e^{-A/2} P = \eta^{-\frac{1}{2}} P$$

and

$$Ph = P\eta^{\frac{1}{2}} H \eta^{-\frac{1}{2}} = \eta^{-\frac{1}{2}} H^* \eta^{\frac{1}{2}} P = hP. \tag{139}$$

In the last part of this section we present another exact approach which is valid only at $g = 1$ for M odd but it exploits the graphical calculus attached to the Temperley–Lieb algebra and is interesting in its own right.

6.1. Example $M = 3$

It might be instructive to start out with the easiest, albeit not the most interesting, case $M = 3$. The non-Hermitian Hamiltonian reads

$$H = -a_{1,2}^- - a_{2,3}^- + ig(n_1 - n_3) \tag{140}$$

where $a_{x,y}^-$ has been defined in (132). The operator $A = \ln \eta$ is then computed to be

$$A = -\frac{\arccos \frac{2+g^2}{2-g^2}}{\sqrt{2}}(a_{1,2}^+ + a_{2,3}^+). \quad (141)$$

After exponentiation, we obtain the quasi-Hermiticity operator and from its explicit form

$$\eta = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{2}{g^2-2} & -\frac{2ig}{g^2-2} & \frac{g^2}{g^2-2} & 0 & 0 & 0 & 0 \\ 0 & \frac{2ig}{g^2-2} & -1 - \frac{4}{g^2-2} & -\frac{2ig}{g^2-2} & 0 & 0 & 0 & 0 \\ 0 & \frac{g^2}{g^2-2} & \frac{2ig}{g^2-2} & -\frac{2}{g^2-2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{2}{g^2-2} & -\frac{2ig}{g^2-2} & \frac{g^2}{g^2-2} & 0 \\ 0 & 0 & 0 & 0 & \frac{2ig}{g^2-2} & -1 - \frac{4}{g^2-2} & -\frac{2ig}{g^2-2} & 0 \\ 0 & 0 & 0 & 0 & \frac{g^2}{g^2-2} & \frac{2ig}{g^2-2} & -\frac{2}{g^2-2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \quad (142)$$

one can explicitly verify that η satisfies all the necessary conditions. Moreover, as predicted from our algebraic analysis related to the $U(\mathfrak{gl}(1|1))$ symmetry of the Hamiltonian, we see that η has a pole precisely at the value $g^2 = (M + 1)/(M - 1) = 2$ where the central element $Z \in U(\mathfrak{gl}(1|1))$ vanishes. The renormalized η ,

$$\eta \rightarrow (g^2 - 2)\eta',$$

still intertwines the Hamiltonian, $\eta' H = H^* \eta'$ at $g^2 = 2$, but is not any longer positive definite but semi-definite. In principle, one can also compute the square root for $\eta^{1/2}$ for general values of g but as the expressions become rather unwieldy we restrict ourselves to stating the result for $g = 1$,

$$\lim_{g \rightarrow 1} \eta^{\frac{1}{2}} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} + \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} & \frac{1}{2} - \frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 \\ 0 & -\frac{i}{\sqrt{2}} & \sqrt{2} & \frac{i}{\sqrt{2}} & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} - \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} & \frac{1}{2} + \frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2} + \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} & \frac{1}{2} - \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 0 & -\frac{i}{\sqrt{2}} & \sqrt{2} & \frac{i}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{2} - \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} & \frac{1}{2} + \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}. \quad (143)$$

After performing the similarity transformation we end up with the Hermitian Hamiltonian

$$\lim_{g \rightarrow 1} h = \frac{a_{1,2}^- + a_{2,3}^-}{\sqrt{2}}. \quad (144)$$

Arguably, we do not see here the manifestation of the long-range nature of the interaction, since the spin-chain is simply too short. However, this case illustrates the working of the general ideas and concepts introduced earlier.

6.2. Example $M = 4$

We saw previously that the cases M even and odd are different and it is therefore important to have another simple but concrete example. We now find

$$A = i \frac{\xi \sqrt{1 + \omega^2}}{2} (a_{1,2}^+ + a_{3,4}^+) + \frac{\xi \zeta + \omega}{2} a_{2,3}^+ + \frac{\xi \zeta - \omega}{2} a_{1,4}^+ \quad (145)$$

where the coefficients are given by

$$\xi = 2 \operatorname{arctanh} \frac{g\sqrt{5-g^2}}{1+g^2+\sqrt{1-g^2}}, \quad \zeta = 2i \operatorname{arctanh} \frac{-1+\sqrt{1-g^2}}{g}, \quad \omega = i\sqrt{\frac{1-g^2}{5-g^2}}. \quad (146)$$

Inserting these expressions into the formula for A does not lead to any further drastic simplifications. Also the expression for the quasi-Hermiticity operator in the spin-sector $S^z = 0$ now looks more complicated: after rescaling

$$\gamma = \sqrt{1-g^2}, \quad \eta' = \gamma(3-g^2-2\gamma)\eta,$$

one finds the matrix

$$\eta' = \begin{pmatrix} 1 & ig & 1-g^2-\gamma & 1-g^2-\gamma & ig(2-g^2-2\gamma) & g^2+2\gamma-2 \\ * & 3-2\gamma & -ig(\gamma-2) & -ig(\gamma-2) & -g^2 & ig(2-g^2-2\gamma) \\ * & * & \gamma-g^2(\gamma-2) & 2-2\gamma & -ig(\gamma-2) & 1-g^2-\gamma \\ * & * & * & \gamma-g^2(\gamma-2) & -ig(\gamma-2) & 1-g^2-\gamma \\ * & * & * & * & 3-2\gamma & ig \\ * & * & * & * & * & 1 \end{pmatrix}. \quad (147)$$

Here we have omitted the lower diagonal part, since $\eta' = \bar{\eta}$. Again one can explicitly check that this operator satisfies all the necessary requirements. From our previous discussion we expect that in the limit $g \rightarrow 1$ the operator η' should cease to be positive definite and become semi-definite. In fact, one verifies that this is the case by using the expression

$$\lim_{g \rightarrow 1} \eta' = \begin{pmatrix} 1 & i & 0 & 0 & i & -1 \\ -i & 3 & 2i & 2i & -1 & i \\ 0 & -2i & 2 & 2 & 2i & 0 \\ 0 & -2i & 2 & 2 & 2i & 0 \\ -i & -1 & -2i & -2i & 3 & i \\ -1 & -i & 0 & 0 & -i & 1 \end{pmatrix}. \quad (148)$$

6.3. Example $M = 5$

Finally, to present one example where the long-range nature at $g = 1$ is slightly more apparent we consider the $M = 5$ chain. We specialize from the start to the case $g = 1$ and find that

$$\lim_{g \rightarrow 1} A = \frac{\xi + \zeta\omega}{2}(a_{1,2}^- + a_{4,5}^-) + \frac{\zeta\sqrt{1-\omega^2}}{\sqrt{2}}(a_{2,3}^- + a_{3,4}^-) + \frac{\xi - \zeta\omega}{2}(a_{1,4}^- + a_{2,5}^-) \quad (149)$$

with

$$\xi = \frac{i \ln 5}{2}, \quad \zeta = i \ln \left[2 + \frac{7}{\sqrt{5}} + 2\sqrt{\frac{16}{5} + \frac{7}{\sqrt{5}}} \right], \quad \omega = \sqrt{\frac{4 + \sqrt{5}}{11}}.$$

After exponentiation we obtain the quasi-Hermiticity operator. In the spin $S^z = 3/2$ sector it reads explicitly

$$\lim_{g \rightarrow 1} \eta = \begin{pmatrix} 1 + \frac{3}{\sqrt{5}} & i + \frac{3i}{\sqrt{5}} & -1 - \frac{1}{\sqrt{5}} & \frac{1}{i\sqrt{5}} - i & 1 \\ \frac{3}{i\sqrt{5}} - i & 1 + \sqrt{5} & i + \frac{3i}{\sqrt{5}} & -1 - \frac{2}{\sqrt{5}} & \frac{1}{i\sqrt{5}} - i \\ -1 - \frac{1}{\sqrt{5}} & \frac{5+3\sqrt{5}}{5i} & 1 + \frac{4}{\sqrt{5}} & i + \frac{3i}{\sqrt{5}} & -1 - \frac{1}{\sqrt{5}} \\ i + \frac{i}{\sqrt{5}} & -1 - \frac{2}{\sqrt{5}} & \frac{5+3\sqrt{5}}{5i} & 1 + \sqrt{5} & i + \frac{3i}{\sqrt{5}} \\ 1 & i + \frac{i}{\sqrt{5}} & -1 - \frac{1}{\sqrt{5}} & \frac{3}{i\sqrt{5}} - i & 1 + \frac{3}{\sqrt{5}} \end{pmatrix} \quad (150)$$

and its square root is computed to be

$$\lim_{g \rightarrow 1} \eta^{\frac{1}{2}} = \begin{pmatrix} \frac{7+9\sqrt[4]{5}-\sqrt{5}+\frac{14}{5^{1/4}}}{22} & \frac{i\sqrt[4]{5}}{2} & \frac{1-5\sqrt[4]{5}+3\sqrt{5}-9/5^{1/4}}{22} & \frac{-i}{2\sqrt[4]{5}} & \frac{7-2\sqrt[4]{5}-\sqrt{5}+\frac{3}{5^{1/4}}}{22} \\ -\frac{i\sqrt[4]{5}}{2} & \frac{\sqrt{4+\sqrt{5}}}{2} & \frac{i}{\sqrt[4]{5}} & \frac{-1}{2\sqrt[4]{5}} & \frac{-i}{2\sqrt[4]{5}} \\ \frac{1-5\sqrt[4]{5}+3\sqrt{5}-\frac{9}{5^{1/4}}}{22} & \frac{-i}{\sqrt[4]{5}} & \frac{4+2\sqrt[4]{5}+\sqrt{5}+8/5^{1/4}}{11} & \frac{i}{\sqrt[4]{5}} & \frac{1-5\sqrt[4]{5}+3\sqrt{5}-\frac{9}{5^{1/4}}}{22} \\ \frac{i}{2\sqrt[4]{5}} & \frac{-1}{2\sqrt[4]{5}} & \frac{-i}{\sqrt[4]{5}} & \frac{\sqrt{4+\sqrt{5}}}{2} & \frac{i\sqrt[4]{5}}{2} \\ \frac{7-2\sqrt[4]{5}-\sqrt{5}+\frac{3}{5^{1/4}}}{22} & \frac{i}{2\sqrt[4]{5}} & \frac{1-5\sqrt[4]{5}+3\sqrt{5}-9/5^{1/4}}{22} & \frac{\sqrt[4]{5}}{2i} & \frac{7+9\sqrt[4]{5}-\sqrt{5}+\frac{14}{5^{1/4}}}{22} \end{pmatrix}. \quad (151)$$

Using these matrix expressions one can compute the Hermitian Hamiltonian h and we find that it is of the expected form,

$$\lim_{g \rightarrow 1} h = \rho_1 (a_{1,2}^- + a_{4,5}^-) + \rho_2 (a_{2,3}^- + a_{3,4}^-) + \rho_3 (a_{1,4}^- + a_{2,5}^-) \quad (152)$$

with

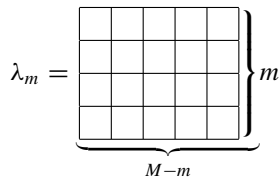
$$\begin{aligned} \rho_1 &= \frac{9 - 6\sqrt{5} - \sqrt{2(15 + 23\sqrt{5})}}{22}, & \rho_2 &= \frac{3 - 2\sqrt{5} - \sqrt{40 + 21\sqrt{5}}}{11}, \\ \rho_3 &= \frac{-2 + 5\sqrt{5} - \sqrt{2(15 + 23\sqrt{5})}}{22}. \end{aligned} \quad (153)$$

The non-local nature of the interaction is now visible in terms of the non-vanishing coefficient ρ_3 . Below we show the result for the spin sector $S^z = 1/2$, however we compute it via different means.

6.4. The quasi-Hermiticity operator and the Temperley–Lieb algebra

In this section we indicate an alternative way to compute the quasi-Hermiticity operator η at $g = 1$ when M is odd employing the Temperley–Lieb algebra. From expressions (74) we expect that in general η will be highly non-local in terms of the spin basis, since the quasi-particle creation and annihilation operators involve sums over the argument of the discrete wavefunctions. Thus, if we compute the matrix elements of η in a fixed spin sector then all elements will be non-vanishing. Our example above for $M = 5$ and $S^z = 3/2$ confirms this, as compared with (150). However, there is another choice of basis in which η simplifies, that is where many of its matrix elements are zero. Namely, we consider the $q \rightarrow i = \sqrt{-1}$ limit of the dual canonical basis [28, 29] which we denote by $\{t_i\}$. The elements of this basis are in one-to-one correspondence with algebra elements $a_i \in TL_M$ and the latter can be written down in terms of Young tableaux; see, e.g. [30].

Fix a spin sector, $S^z = \text{const}$, and set $m = M/2 - S^z$. Let λ_n be the rectangular Young diagram with n rows of $N - n$ boxes,



Then we assign to each subdiagram $\lambda' \subset \lambda_m$ a vector as follows. Let t be the unique standard tableau (column and row strict) of shape λ' whose entries are consecutive integers with entry n in the upper-left corner. For example,

$$t = \begin{array}{|c|c|c|c|c|} \hline m & m+1 & m+2 & \dots & s \\ \hline m-1 & m & \dots & s-2 & \\ \hline \vdots & & & & \\ \hline s' & & & & \\ \hline \end{array}, \quad m < s < M, \quad 1 \leq s' < m. \quad (154)$$

Reading the entries of the tableau from left to right and top to bottom we set

$$t \mapsto e_{s'} e_{s'-1} \dots e_{s-2} \dots e_{m-1} e_s \dots e_{m+1} e_m \Omega_m, \quad (155)$$

where

$$\Omega_m = \underbrace{v_- \otimes v_- \dots \otimes v_-}_m \otimes v_+ \otimes v_+ \dots \otimes v_+ \quad (156)$$

is the vector corresponding to $\lambda' = \emptyset$. Note that for fixed m there are as many of these tableaux as the dimension of the spin sector, namely $\binom{M}{m}$.

Example. Let $M = 5$ and $m = 2$ then we have the following Young diagrams and tableaux:

$$t = \emptyset, \quad \boxed{2}, \quad \begin{array}{|c|} \hline 2 \\ \hline 1 \\ \hline \end{array}, \quad \boxed{2} \boxed{3}, \quad \begin{array}{|c|c|} \hline 2 & 3 \\ \hline 1 & \\ \hline \end{array}, \quad \begin{array}{|c|c|c|} \hline 2 & 3 & 4 \\ \hline 1 & & \\ \hline \end{array}, \quad \begin{array}{|c|c|c|c|} \hline 2 & 3 & 4 & \\ \hline 1 & & & \\ \hline \end{array}, \quad \begin{array}{|c|c|c|} \hline 2 & 3 & 4 \\ \hline 1 & 2 & \\ \hline \end{array}, \quad \begin{array}{|c|c|c|} \hline 2 & 3 & 4 \\ \hline 1 & 2 & 3 \\ \hline \end{array}.$$

The corresponding algebra elements $a \in TL_M(q)$ are

$$a = 1, e_2, e_1 e_2, e_3 e_2, e_4 e_3 e_2, e_1 e_3 e_2, e_2 e_1 e_3 e_2, e_1 e_4 e_3 e_2, e_2 e_1 e_4 e_3 e_2, e_3 e_2 e_1 e_4 e_3 e_2.$$

Each of these algebra elements we can also represent as a link or Kauffman diagram. Identifying

$$e_i = \begin{array}{c} \left| \dots \right| \begin{array}{c} \cup \\ \cap \end{array} \left| \dots \right| \\ i \quad i+1 \end{array}$$

and realizing multiplication by concatenation from above, we find the following diagrams for the algebra elements,

$a \in TL_5$	$a_1 = 1$	$a_2 = e_2$	$a_3 = e_1 e_2$	$a_4 = e_3 e_2$	$a_5 = e_4 e_3 e_2$	$a_6 = e_1 e_3 e_2$
diagram						

and

$a \in TL_5$	$a_7 = e_2 e_1 e_3 e_2$	$a_8 = e_1 e_4 e_3 e_2$	$a_9 = e_2 e_1 e_4 e_3 e_2$	$a_{10} = e_3 e_2 e_1 e_4 e_3 e_2$
diagram				

We will make use of these diagrams momentarily. Employing the representation $TL_M \rightarrow \text{End } V^{\otimes M}$ introduced earlier,

$$e_x \mapsto c_x c_{x+1}^* - c_x^* c_{x+1} + i(n_x - n_{x+1}),$$

we can now generate the basis vectors t_i by acting with each corresponding algebra element a_i onto the vector Ω_m . Computing from our previous expression (74) the quasi-Hermiticity

operator η we can evaluate its matrix elements in this new basis. Based on numerical computations for $M = 3, 5, 7$ we arrive at the following conjecture.

Conjecture 6. Denote by G the Gram matrix of the dual canonical basis vectors $\{t_i\}$ with respect to the η -product, i.e.

$$G_{ij} = \langle t_i, \eta t_j \rangle.$$

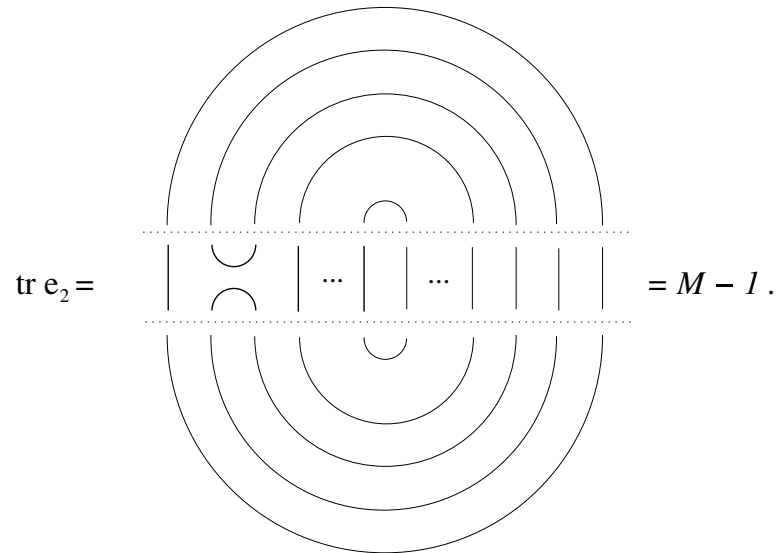
Then we have

$$G_{ij} = 0 \quad \text{whenever} \quad \text{tr}(a_i a_j) = 0 \pmod 2,$$

where a_i, a_j are the algebra elements corresponding to t_i, t_j and

$$\text{tr } a = \text{tr } a e_M = \text{number of closed loops}$$

which are obtained by closing the planar diagram associated with a . An example for $a = e_2$ is shown below:



Remark. Note that the above relation does not necessarily imply that $G_{ij} \neq 0$ if $\text{tr}(a_i a_j) = 1 \pmod 2$. The Gram matrix inherits from η the further properties

$$\det G = 1, \quad G > 0 \quad \text{and} \quad G_{ij} = G_{ji} \in \mathbb{R}.$$

Knowledge of the Gram matrix is sufficient to compute matrix elements with respect to the η -product. In particular, the intertwining property, $\eta H = H^* \eta$, translates into the following identity for the Gram matrix

$$G \mathcal{H} = \mathcal{H}' G, \tag{157}$$

where the matrix \mathcal{H} has only integer entries, $\mathcal{H}_{ji} \in \mathbb{Z}$, and is defined via

$$H t_i = \sum_j t_j \mathcal{H}_{ji}. \tag{158}$$

Note that \mathcal{H} can be computed graphically using link diagrams. For instance, we find for our example $M = 5$ and $S^z = 1/2$ stated above that

$$\mathcal{H} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 2 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}. \tag{159}$$

The corresponding Gram matrix is

$$G = \begin{pmatrix} \frac{2(3+\sqrt{5})}{5} & 0 & \frac{2(1+\sqrt{5})}{5} & \frac{3}{5} + \frac{1}{\sqrt{5}} & 0 & 0 & -\frac{2}{5} & \frac{2}{5} & 0 & \frac{3}{5} \\ 0 & 1 + \frac{3}{\sqrt{5}} & 0 & 0 & 1 + \frac{1}{\sqrt{5}} & 0 & 0 & 0 & 1 & 0 \\ \frac{2(1+\sqrt{5})}{5} & 0 & \frac{2(2+\sqrt{5})}{5} & \frac{1}{5} + \frac{1}{\sqrt{5}} & 0 & 0 & \frac{1}{5} & \frac{4}{5} & 0 & \frac{1}{5} \\ \frac{3}{5} + \frac{1}{\sqrt{5}} & 0 & \frac{1}{5} + \frac{1}{\sqrt{5}} & \frac{3(3+\sqrt{5})}{5} & 0 & 0 & \frac{4}{5} & \frac{1}{5} & 0 & \frac{9}{5} \\ 0 & 1 + \frac{1}{\sqrt{5}} & 0 & 0 & 1 + \frac{2}{\sqrt{5}} & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ -\frac{2}{5} & 0 & \frac{1}{5} & \frac{4}{5} & 0 & 0 & \frac{9}{5} & \frac{1}{5} & 0 & \frac{4}{5} \\ \frac{2}{5} & 0 & \frac{4}{5} & \frac{1}{5} & 0 & 0 & \frac{1}{5} & \frac{4}{5} & 0 & \frac{1}{5} \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\ \frac{3}{5} & 0 & \frac{1}{5} & \frac{9}{5} & 0 & 0 & \frac{4}{5} & \frac{1}{5} & 0 & \frac{9}{5} \end{pmatrix}. \tag{160}$$

One can check that the above conjecture holds true for this example using the stated link diagrams.

In addition to identity (157) we obtain further constraints on the Gram matrix by employing PT invariance, $\eta^{-1} = P\eta P = \bar{\eta} = \eta^t$, from which we conclude that

$$G_{ij} = \langle Tt_i, \eta^{-1}Tt_j \rangle$$

and hence

$$\mathcal{M}^*G\mathcal{M} = G, \quad PTt_i = \sum_j t_j \mathcal{M}_{ji}. \tag{161}$$

It is desirable to find a closed formula for the Gram matrix elements similar to the case treated in [21, 22].

7. Results for boundary fields off the imaginary axis

In this section we briefly discuss some aspects when $\alpha = \bar{\beta}$ do not lie on the imaginary axis. This case for $\alpha = \bar{\beta}$ on the unit circle has been investigated previously [13, 33, 14] albeit not in the context of quasi-Hermiticity. Here we relate our discussion to these previous results.

7.1. $U_q(\mathfrak{gl}(1|1))$ invariance and the Hecke algebra

In order to discuss the quantum group symmetry we consider the Hamiltonian H' instead of H ,

$$H' = \sum_{m=1}^M H'_m, \quad H'_m = -\frac{\sigma_m^x \sigma_{m+1}^x + \sigma_m^y \sigma_{m+1}^y - \alpha^{-1} \sigma_m^z - \alpha \sigma_{m+1}^z}{2}.$$

This Hamiltonian can be viewed as an element in the Hecke Algebra, as compared with the discussion in [31, 33].

Definition 4. The Hecke algebra $\mathcal{H}_n(q)$ with $q \in \mathbb{C}$ is the associative algebra (over \mathbb{C}) obtained from the generators b_1, \dots, b_{n-1} subject to the relations

$$b_i b_i^{-1} = b_i^{-1} b_i = 1, \quad b_j b_{j+1} b_j = b_{j+1} b_j b_{j+1}, \quad b_i b_j = b_j b_i \quad \text{for } |i - j| > 1$$

and

$$b_i^2 + (q - q^{-1})b_i = 1.$$

Setting $n = M$ and $q = -\alpha^{-1}$ one easily verifies that

$$b_i \mapsto c_i c_{i+1}^* - c_i^* c_{i+1} - \alpha^{-1} n_i - \alpha(n_{i+1} - 1) = \begin{pmatrix} q & 0 & 0 & 0 \\ 0 & q - q^{-1} & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -q^{-1} \end{pmatrix}_{i,i+1}$$

and

$$b_i^{-1} \mapsto c_i c_{i+1}^* - c_i^* c_{i+1} - \alpha^{-1}(n_i - 1) - \alpha n_{i+1} = \begin{pmatrix} -q^{-1} & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & q^{-1} - q & 0 \\ 0 & 0 & 0 & q \end{pmatrix}_{i,i+1}$$

yield a representation of the Hecke algebra $\mathcal{H}_M(q = -\alpha^{-1})$ over $V^{\otimes M}$ and, furthermore, we have the identity

$$H' = \sum_{i=1}^{M-1} \frac{b_i + b_i^{-1}}{2}. \tag{162}$$

There is the action of the quantum group $\mathcal{U}_q(\mathfrak{gl}(1|1))$ [31, 32] which is ‘dual’ to the action of the Hecke algebra in the sense that both of them commute, i.e. the Hamiltonian is quantum group invariant.

Definition 5. Consider the associative algebra $\mathcal{U}_q(\mathfrak{gl}(1|1))$ over $\mathbb{C}(q)$ generated by the elements $\{\mathcal{X}^\pm, \mathcal{Y}^{\pm 1}, \mathcal{Z}^{\pm 1}\}$ subject to the relations

$$\mathcal{Z} \mathcal{Z}^{-1} = \mathcal{Z}^{-1} \mathcal{Z} = \mathcal{Y} \mathcal{Y}^{-1} = \mathcal{Y}^{-1} \mathcal{Y} = 1, \quad \mathcal{Y} \mathcal{X}^\pm \mathcal{Y}^{-1} = q^{\pm 1} \mathcal{X}^\pm, \quad [\mathcal{Y}, \mathcal{Z}] = [\mathcal{Z}, \mathcal{X}^\pm] = 0 \tag{163}$$

and

$$[\mathcal{X}^\pm, \mathcal{X}^\pm]_+ = 0, \quad [\mathcal{X}^+, \mathcal{X}^-]_+ = \frac{\mathcal{Z} - \mathcal{Z}^{-1}}{q - q^{-1}}. \tag{164}$$

Setting $q = -\alpha^{-1}$ and identifying

$$\mathcal{Y}^{\pm 1} \mapsto q^{\pm S^z}, \quad \mathcal{Z}^{\pm 1} \mapsto q^{\pm M}, \quad \mathcal{X}^+ \mapsto \sum_x q^{\frac{M+1}{2}-x} c_x^*, \quad \mathcal{X}^- \mapsto \sum_x q^{\frac{M+1}{2}-x} c_x,$$

we obtain a representation of this algebra over $V^{\otimes M}$. Moreover, its action commutes with the action of the Hecke algebra,

$$[\mathcal{U}_q(\mathfrak{gl}(1|1)), \mathcal{H}_M(q)] = 0,$$

and, thus, with the Hamiltonian H' . As before the quantum group invariance is reflected in the existence of a particularly simple solution for the discrete wavefunction. Setting as before $q = -\alpha^{-1} = e^{i\theta}$ the mentioned wavefunction and creation operator are

$$\psi_\theta(x) = \sqrt{\frac{\sin \theta}{\sin M\theta}} e^{i(x - \frac{M+1}{2})\theta}, \quad \hat{c}_\theta^* = \sqrt{\frac{\sin \theta}{\sin M\theta}} \mathcal{X}^+ = \sum_{x=1}^M \psi_\theta(x) c_x^*. \quad (165)$$

Using these expressions one finds

$$[H, \hat{c}_\theta^*] = -2 \cos \theta \hat{c}_\theta^* \quad \text{and} \quad [H', \hat{c}_\theta^*] = 0. \quad (166)$$

Similar as in the case $\theta = \pi/2$ and M even the Hamiltonian has non-trivial Jordan blocks when the norm of the wavefunction becomes singular, that is if we choose θ such that

$$\frac{\sin M\theta}{\sin \theta} = 0.$$

Also the representation theoretic interpretation of η extends from $\theta = i\pi/2$ to the present, general case: the new inner product $\langle \cdot, \eta \cdot \rangle$ gives rise to a representation of the quantum group $\mathcal{U}_q(\mathfrak{gl}(1|1))$ with the correct $*$ -structure,

$$\eta \mathcal{X}^+ = (\mathcal{X}^-)^* \eta. \quad (167)$$

The above identity has another consequence. Since we also have that $P \mathcal{X}^+ P = (\mathcal{X}^-)^*$ it follows that the C -operator obeys

$$[C, \mathcal{U}_q(\mathfrak{gl}(1|1))] = 0, \quad C = P \eta$$

and hence must be an element in the Hecke algebra. This is precisely the line of reasoning employed in [11] to find an algebraic expression for C . However, we need an additional ingredient to complete the analogous computation: the decomposition of the state space into $\mathcal{U}_q(\mathfrak{gl}(1|1))$ -modules [34]. We leave this problem to future work.

7.2. Perturbation theory for arbitrary θ

In this section we wish to confirm that our previous picture for $\theta = \pi/2$ stays intact for general θ . Namely, we wish to show that also here the non-Hermitian boundary fields in H, H' correspond to non-local hopping terms in h .

For arbitrary θ we have to modify our previous approach to the perturbative computation of $\eta = \exp A$. We now define

$$\alpha = \beta^* = -g e^{i\theta}, \quad 0 \leq g < 1 : H_g = H_0 + g H_1$$

with

$$H_0 = - \sum_{x=1}^{M-1} [c_x^* c_{x+1} - c_x c_{x+1}^*], \quad H_1 = - \frac{e^{i\theta} \sigma_1^z + e^{-i\theta} \sigma_M^z}{2} = -(e^{i\theta} n_1 + e^{-i\theta} n_M). \quad (168)$$

For $0 < g \ll 1$ we again expand the operator $\eta = \exp A$ using the Baker–Campbell–Hausdorff formula but now we cannot make the ansatz that A only depends on odd powers of the coupling constant g , since $H_g^* \neq H_{-g}$. Thus, all powers of g are occurring in the series expansion,

$$A = \sum_{n>0} g^n A_n. \quad (169)$$

Collecting once more terms of the same order in g we now arrive at

$$\begin{aligned} [H_0, A_1] &= 2H_-, \\ [H_0, A_2] &= [A_1, H_1] + \frac{1}{2}[A_1, [A_1, H_0]] = [A_1, H_+], \\ [H_0, A_3] &= [A_2, H_+] - \frac{1}{12}[A_1, [A_1, [A_1, H_0]]] = [A_2, H_+] + \frac{1}{6}[A_1, [A_1, H_-]], \end{aligned} \tag{170}$$

where

$$H_+ = \frac{H_1 + H_1^\dagger}{2} = -\cos \theta(n_1 + n_M) \quad \text{and} \quad H_- = \frac{H_1 - H_1^\dagger}{2} = i \sin \theta(n_M - n_1). \tag{171}$$

The explicit results for the first two terms in the expansion of the matrix A are

$$\begin{aligned} A_1 &= \sum_{x=1}^{M-1} [e^{i\theta} c_x^* c_{x+1} - e^{-i\theta} c_x c_{x+1}^*], \\ A_2 &= \sum_{x=1}^{M-2} [(1 + e^{2i\theta}) c_x^* c_{x+2} - (1 + e^{-2i\theta}) c_x c_{x+2}^*]. \end{aligned}$$

The corresponding Hermitian Hamiltonian h now reads up to third order in the coupling g ,

$$h = e^{\frac{A}{2}} H e^{-\frac{A}{2}} = H_0 + \sum_{n=1}^{\infty} g^n h_n,$$

with

$$\begin{aligned} h_1 &= H_+ = -\cos \theta(n_1 + n_M), \\ h_2 &= \frac{1}{4}[A_1, H_-] = \frac{\sin \theta}{4i} e^{i\theta} (c_1^* c_2 + c_{M-1}^* c_M) + \text{h.c.}, \\ h_3 &= \frac{1}{4}[A_2, H_-] = \frac{\sin \theta}{4i} (1 + e^{i2\theta}) (c_1^* c_3 + c_{M-2}^* c_M) + \text{h.c.} \end{aligned}$$

Here, ‘h.c.’ stands for the Hermitian conjugate of the previous term. From this we infer that for general values of θ also interactions between sites separated by an even number are possible.

8. Conclusions

In this paper we encountered numerous new aspects of the XX spin-chain with non-Hermitian boundary fields. While this simple integrable model has been studied intensively before in the literature, it has recently received renewed attention because of its possible connection with logarithmic conformal field theories. The suggestion in [7, 8] is that lattice systems, such as the non-Hermitian XX spin-chain, might be used to gain insight into logarithmic CFTs (see, e.g. [9, 10]) via representations of the Temperley–Lieb algebra with non-trivial Jordan blocks.

The present work has highlighted a very different aspect: purely on physical grounds one wishes to have a Hermitian quantum Hamiltonian (without Jordan blocks) in order to ensure a unitary time evolution of the system. This is one of the essential demands of quantum mechanics. We have seen that this can be achieved for complex boundary fields with values inside the unit disc via two different, albeit closely related routes: one can either introduce a new inner product or perform a similarity transformation to a Hermitian Hamiltonian. The latter leads to a new physical interpretation of the non-Hermitian XX spin-chain: it corresponds to a free fermion system with long-range hopping. The probability of long-range hopping taking place is controlled by the absolute value of the complex boundary fields. This new perspective on the XX spin-chain with non-Hermitian boundary fields entails a range of other

physically interesting questions, such as finite size effects and correlation functions. We already touched upon the finite size scaling of the groundstate energy in the text, since the latter contains information about the respective CFTs in the thermodynamic limit and thus would connect with the discussion in [6–8]. Due to the absence of an exact solution for the Bethe roots when the boundary fields lie within the unit disc, we were unable to obtain conclusive results. An alternative approach might be to find a field-theoretic model which allows one to compute the partition function, similar as it has been the case for critical dense polymers on the lattice [6].

To find the correct field-theoretic counterpart might be facilitated by the algebraic structures pointed out in this paper. We explicitly constructed representations of the quantum group $U_q(\mathfrak{sl}_2)$ with $q = \sqrt{-1}$ and the superalgebra $U(\mathfrak{gl}(1|1))$ which can be extended from the unit circle along the imaginary axis. Any field theory describing the thermodynamic limit should reflect these algebraic features. Recall that for M odd these algebras provided symmetries, while they did not for M even. Our careful analysis showed that we could tie the appearance of (non-trivial) Jordan blocks in the Hamiltonian to the vanishing of the central element among the generators of $U(\mathfrak{gl}(1|1))$. For M even this happens precisely if the boundary fields lie on the unit circle, but the new result here is that it also happens for M odd just outside the unit circle. Moreover, we recall from the main text that for M even one obtains 2×2 Jordan blocks, while for M odd one has 3×3 blocks. Thus, the algebraic picture put forward in [8] for M even needs to be modified for M odd and an interesting problem is whether one can find also here corresponding logarithmic CFTs.

The superalgebra $U(\mathfrak{gl}(1|1))$ has also been connected to the discussion of quasi-Hermiticity. The new inner product preserves the natural $*$ -involution of $U(\mathfrak{gl}(1|1))$, thus providing a representation-theoretic interpretation of our construction. It is this feature which singles out non-Hermitian quantum integrable systems: due to their underlying algebraic structures they allow for various interpretations and *exact* constructions of the quasi-Hermiticity operator. This connection between abstract mathematical structures and physically motivated concepts such as PT symmetry is mutually beneficial, it leads to new physical insight and interesting mathematical questions even for a simple and well-studied model such as the XX spin-chain.

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